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New compounds for the inhibition of rotamases and use thereof

The present invention is related to new compounds and the use of said compounds as an inhibitor to rotamases and for the manufacture of medicaments.

Rotamases, also referred to as peptidyl-prolyl cis-trans isomerases (PPIases) are a family of enzymes important in protein folding, assembly and transport. They act as catalysts to promote isomerization about the peptidyl-prolyl bond, which can have profound effects on protein function.

PPIases are divided into three classes, cyclophilins, FK-506 binding proteins (FKBPs) and the Pin1/parvulin class. While cyclophilins and FKBPs are distinguished by their ability to bind immunosuppressant molecules cyclosporin and FK-506, respectively, the Pin1/parvulin class binds neither of these immunosuppressants and is structurally unrelated to the other two classes. Known members of the Pin1/parvulin class include Pins 1 – 3 (Lu et al., Nature 380:544-547, 1996), Pin-L (Campbell et al., Genomics 44:157-162, 1997), parvulin (Rahfeld et al., FEBS Letts 352:180-184, 1994), dodo (Maleszka et al., Proc Natl Acad Sci USA 93:447-451, 1996) and Ess1/Pft1 (Hanes et al., Yeast 5:55-72, 1989; and Hani et al., FEBS Letts 365:198-202, 1995).

Recent research suggests that members of the Pin1/parvulin class are essential modulators of the cell cycle, and mitosis in particular. Lu et al., Nature 380:544-547, 1996 reports that depletion of Pin1/Ess1 in yeast or human cells induces mitotic arrest followed by apoptosis, indicating that enzymes in this class serve an essential function in cell division and proliferation.

Accordingly, compounds inhibiting rotamases can serve as agents for the treatment of a variety of disorders which are characterized by an inappropriate cell proliferation including cancer and infectious diseases.

In the prior art a huge number of compounds are described which are active as inhibitors to rotamase. The respective compounds are, among others, peptide derivatives such as amino methylene-peptides which are described in European patent EP 0 610 743, or non-peptidic or non-peptidomimetic molecules.

Given the importance of rotamase there is an ongoing need in the art to provide further compounds which are suitable as inhibitors to rotamases and thus suitable to be used as a medicament for those diseases wherein a rotamase is involved in the pathological mechanism.

Accordingly, the problem underlying the present invention is to provide compounds which inhibit a rotamase. A further problem underlying the present invention is to provide new compounds for the treatment of diseases the pathophysiology of which involves an imbalanced or undesired activity of a rotamase.

In a first aspect the problem underlying the present invention is solved by a compound having the structure

$$A-[X]_{t}-Y \qquad (0)$$

wherein A is selected from the group comprising cycloalkyl, substituted cycloalkyl, heterocyclyl, substituted heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl;

X is a spacer and is independently selected from the group comprising

-M1-L1-K-L2-M2-,

$$-M_1-L_1-K-L_2-M_2-$$
,  $-M_1-L_1-K-L_2-M_2-$ ,  $-M_1-L_1-K-L_2-M_2-$ ,  $-M_1-L_1-K-L_2-M_2-$ 

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wherein K is selected from the group comprising

C=T,

O, S, S(O) and  $S(O_2)$ ,

or is absent,

with =T being selected from the group comprising

=O, =S, =N-R°, =N-CN, =N-NO<sub>2</sub> and =CH-NO<sub>2</sub>.

L1 and L2 are each and independently selected from the group comprising O, S and primary amines, more particularly NR<sup>c</sup>, NR<sup>d</sup>; or being individually and independent from each other absent

M1 and M2 are each and independently selected from the group comprising

 $-(CR^aR^b)n-$ ,

 $-(CR^fR^g)m-,$ 

cycloalkyl, substituted cycloakyl, heterocyclyl, substituted heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl heteroaryl, or being individually and independent from each other absent,

wherein t is independently selected from n and/or m and is any integer from 0 to 10, whereby if t is 2 or more any of the spacer -M1-L1-K-L2-M2- can be the same or different from any of the spacer(s) X repeated,

wherein R<sup>c</sup>, R<sup>d</sup> and R<sup>e</sup> are independently from each other selected from the group H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl;

wherein R<sup>a</sup>, R<sup>b</sup>, R<sup>f</sup> and R<sup>g</sup> are independently from each other selected from the group H, OR<sub>17</sub>, SR<sub>18</sub>, NR<sub>19</sub>R<sub>20</sub>, halo, alkyl, substituted alkyl, alkylaryl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl,

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heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl; or may be independently from each other absent, and

wherein Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkynyl, substituted branched alkynyl, cycloalkyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl,

or wherein Y is absent.

In a preferred embodiment Y is different from a peptide.

In a further embodiment A is

$$R_{1}$$
- $Z_{1}$ 
 $R_{5}$ 
 $R_{3}$ - $Z_{3}$ 
 $Z_{4}$ - $Z_{4}$ 
 $Z_{4}$ - $Z_{4}$ 

$$R_{1}$$
- $Z_{1}$ 
 $R_{5}$ 0
 $Z_{4}$ - $Z_{4}$ 
 $Z_{4}$ - $Z_{4}$ 
 $Z_{4}$ - $Z_{4}$ 
 $Z_{4}$ - $Z_{4}$ 

In a second aspect which is actually an embodiment of the first aspect of the invention, the problem is solved by a compound which has any of the structures according to formulae (I), (III), (IV) or (V):

wherein R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> and R<sub>4</sub> are each independently selected from the group comprising H, OR<sub>6</sub>, SR<sub>7</sub>, NR<sub>8</sub>R<sub>9</sub>, halo, alkyl, substituted alkyl, alkylaryl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl;

wherein  $R_1$  and  $R_2$ ,  $R_2$  and  $R_3$ ,  $R_3$  and  $R_4$ ,  $R_1$  and  $R_3$ ,  $R_1$  and  $R_4$ , and  $R_2$  and  $R_4$  may be linked so as to form a ring comprising 4 to 12 members, preferably 5 to 10 members, more preferably 5 or 6 or 7 members,

wherein  $Z_1$ ,  $Z_2$ ,  $Z_3$  and  $Z_4$  are each and independently selected from the group comprising – C(O)–, –C(S)–, –C(O)– $NR_{10}$ -, –C(S)– $NR_{11}$ -, –C(N–CN)– $NR_{12}$ -, –S(O)-, –S(O)– $NR_{13}$ -, – $S(O_2)$ – $NR_{14}$ -, –O–, and –S–, or are each and individually absent;

R<sub>5</sub> is selected from the group comprising H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl, substituted alkylheteroaryl and -C(O)-Q;

wherein Q is selected from the group comprising H, NHR<sub>15</sub>, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl, and substituted alkylheteroaryl; and

R<sub>6</sub>, R<sub>7</sub>, R<sub>8</sub>, R<sub>9</sub>, R<sub>10</sub>, R<sub>11</sub>, R<sub>12</sub>, R<sub>13</sub>, R<sub>14</sub> and R<sub>15</sub> are each and independently selected from the group comprising H, alkyl, substituted alkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, alkoxy, substituted alkoxy, aryloxy, substituted aryloxy, alkylamino, substituted alkylamino, arylamino and substituted arylamino;

X is a spacer and is independently selected from the group comprising

-M1-L1-K-L2-M2-,

wherein K is selected from the group comprising

C=T.

O, S, S(O) and  $S(O_2)$ ,

or is absent,

with =T being selected from the group comprising

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L1 and L2 are each and independently selected from the group comprising O, S and primary amines, more particularly NR<sup>c</sup>, NR<sup>d</sup>; or being individually and independent from each other absent

M1 and M2 are each and independently selected from the group comprising  $-(CR^aR^b)n$ -,

 $-(CR^fR^g)m-,$ 

cycloalkyl, substituted cycloakyl, heterocyclyl, substituted heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl heteroaryl, or being individually and independent from each other absent,

wherein D is  $C_1$ – $C_6$  alkyl, preferably straight  $C_1$ – $C_6$  alkyl,  $C_1$ – $C_6$  alkenyl, preferably straight  $C_1$ – $C_6$  alkynyl, whereby preferably any of the alkyl, alkenyl and alkynyl may individually and independently comprise from 0 to 3 heteroatoms, and/or whereby preferably any of the alkyl, alkenyl and alkynyl can be individually and independently substituted, more preferably by 1 or 2 substituent(s) preferably each independently selected from H, halo,  $OR_{16}$ , alkyl, and substituted alkyl,

wherein n and m are each and independently selected from each other and are each any integer from 0 to 10,

whereby if n is 2 or more, the group(s) –(CR<sup>a</sup>R<sup>b</sup>)– which is/are repeated, can be the same or different from any of the group(s) –(CR<sup>a</sup>R<sup>b</sup>)–,

whereby any individual group can be linked to any other group or any moiety of the compound through a bond selected from the group comprising single bonds, double bonds and triple bonds,

whereby if m is 2 or more, the group(s) -(CR<sup>f</sup>R<sup>g</sup>)- which is/are repeated, can be the same or different from any of the group(s) -(CR<sup>f</sup>R<sup>g</sup>)-,

whereby any individual group can be linked to any other group or any moiety of the compound through a bond selected from the group comprising single bonds, double bonds and triple bonds,

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wherein t is independently selected from n and/or m and is any integer from 0 to 10, whereby if t is 2 or more any of the spacer -M1-L1-K-L2-M2- can be the same or different from any of the spacer(s) X repeated,

## wherein

R<sup>c</sup>, R<sup>d</sup> and R<sup>e</sup> are independently from each other selected from the group H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted heterocyclyl, alkylheterocyclyl, beteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl; and

R<sup>a</sup>, R<sup>b</sup>, R<sup>f</sup> and R<sup>g</sup> are independently from each other selected from the group H, OR<sub>17</sub>, SR<sub>18</sub>, NR<sub>19</sub>R<sub>20</sub>, halo, alkyl, substituted alkyl, alkylaryl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl; or may be independently from each other absent, and

wherein E is  $C_1$ – $C_6$  alkyl, preferably straight  $C_1$ – $C_6$  alkyl,  $C_1$ – $C_6$  alkenyl, preferably straight  $C_1$ – $C_6$  alkenyl,  $C_1$ – $C_6$  alkynyl, preferably straight  $C_1$ – $C_6$  alkynyl, whereby preferably any of the alkyl, alkenyl and alkynyl may comprise individually and independently from 0 to 3 heteroatoms, and/or whereby preferably any of the alkyl, alkenyl and alkynyl can be individually and independently substituted by preferably 1 or 2 substituent(s) each preferably independently selected from the group comprising H, halo,  $OR_{21}$ , alkyl, and substituted alkyl.

R<sub>16</sub>, R<sub>17</sub>, R<sub>18</sub>, R<sub>19</sub>, R<sub>20</sub> and R<sub>21</sub> are each and independently selected from the group comprising H, alkyl, substituted alkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, alkoxy, substituted alkoxy, aryloxy, substituted aryloxy, alkylamino, substituted alkylamino, arylamino and substituted arylamino;

wherein Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl,

substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkynyl, substituted branched alkynyl, cycloalkyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl,

or wherein Y is absent.

In an embodiment Y is different from a peptide.

In an embodiment of the first and the second aspect of the present invention the moiety A and phenol moiety, respectively forms a cyclic structure with the spacer X and/or Y.

In an embodiment of the first and the second aspect of the present invention the compound is

$$R_{1}-Z_{1}$$

$$R_{2}-Z_{2}$$

$$R_{3}-Z_{3}$$

$$R_{1}-Z_{1}$$

$$R_{2}-Z_{2}$$

$$R_{3}-Z_{3}$$

$$R_{1}-Z_{1}$$

$$R_{2}-Z_{2}$$

$$R_{3}-Z_{3}$$

$$R_{1}-Z_{1}$$

$$R_{2}-Z_{2}$$

$$R_{1}-Z_{1}$$

$$R_{2}-Z_{2}$$

$$R_{1}-Z_{1}$$

$$R_{2}-Z_{2}$$

$$R_{2}-Z_{2}$$

$$R_{2}-Z_{2}$$

$$R_{3}-Z_{4}$$

$$R_{4}-Z_{1}$$

$$R_{2}-Z_{2}$$

$$R_{4}-R_{4}$$

$$R_{2}-Z_{2}$$

$$R_{4}-R_{4}$$

$$R_{2}-Z_{2}$$

$$R_{4}-R_{4}$$

$$R_{2}-Z_{2}$$

In a further embodiment of the first and the second aspect of the present invention the compound is selected from the group comprising

In an embodiment of the first and the second aspect of the present invention K is C=T.

In a further embodiment of the first and the second aspect of the present invention T is selected from the group comprising O and S.

In a preferred embodiment of the first and the second aspect of the present invention T is O.

In an alternative preferred embodiment of the first and the second aspect of the present invention T is S.

In a further alternative embodiment of the first and the second aspect of the present invention. T is selected from the group comprising N-CN, N-NO<sub>2</sub>, CH-NO<sub>2</sub> and N-R<sup>e</sup>.

In an embodiment of the first and the second aspect of the present invention, more particularly the embodiment where T is either O or S, L1 and L2 are each and independently a primary amine, preferably NR<sup>c</sup> and/or NR<sup>d</sup>.

In an embodiment of the first and the second aspect of the present invention n = 0 and m is any integer from 0 to 10.

In an embodiment of the first and the second aspect of the present invention  $R_1$  and/or  $R_3$  are selected from the group comprising halo, alkyl, substituted alkyl, heterocyclyl, substituted heterocyclyl, heterocyclyl and substituted heterocyclyl. In an even more preferred embodiment  $R_1$  is halo.

In an embodiment of the first and the second aspect of the present invention  $R_5$  is selected from the group comprising H and -C(O)-Q. In a preferred embodiment Q is selected from alkylheterocyclyl and substituted alkylheterocyclyl. In an even more preferred embodiment Q is selected from the group comprising N-acylated morpholino-, N-acylated piperazino- and N-acyl-derivatives.

In an embodiment of the first and the second aspect of the present invention R<sub>6</sub> is alkyl or substituted alkyl.

In an embodiment of the first and the second aspect of the present invention  $R_8$  and  $R_9$  are individually and separately selected from the group comprising H, alkyl and substituted alkyl.

In an embodiment of the first and the second aspect of the present invention n and m are individually and independently any integer from 1 to 3.

In an alternative embodiment of the first and the second aspect of the present invention n is any integer from 0 to 3 and is preferably 0 or 1.

In a further alternative embodiment of the first and the second aspect of the present invention n and m are both 0.

In an embodiment of the first and the second aspect of the present invention t is 1 or 2.

In another embodiment of the first and the second aspect of the present invention R<sup>c</sup> and/or R<sup>d</sup> are each and independently from each other selected from the group comprising alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl.

In still another embodiment of the first and the second aspect of the present invention  $R^a$ ,  $R^b$ ,  $R^f$  and  $R^g$  are each individually and independently from each other selected from the group comprising H,  $OR_{17}$ ,  $SR_{18}$ ,  $NR_{19}R_{20}$ , halo, alkyl and substituted alkyl.

In a preferred embodiment of the first and the second aspect of the present invention Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkylnyl and substituted branched alkynyl.

In an alternate preferred embodiment of the first and the second aspect of the present invention Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, monounsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or is absent.

In a particularly preferred embodiment of the first and the second aspect of the present invention which is also referred to as the NR-CZ-NR embodiment X is

$$-(CR^aR^b)_n-NR^c-CZ-NR^d-(CR^fR^g)_m-$$

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and Z is preferably selected from the group comprising O, S, N-CN, N-NO2 and CH-NO2.

In an embodiment of the NR-CZ-NR embodiment m is any integer from 1 to 10.

In an embodiment of the NR-CZ-NR embodiment  $R_5$  is selected from the group comprising H and -C(O)-Q, preferably m is any integer from 1 to 10.

In an embodiment of the NR-CZ-NR embodiment wherein R<sub>5</sub> is H.

In an embodiment of the NR-CZ-NR embodiment n is 0, preferably  $R_5$  being selected from the group comprising H and -C(O)-Q, more preferably m being any integer from 1 to 10. In an alternative embodiment n is any integer from 1 to 10.

In an embodiment of the NR-CZ-NR embodiment t is 1.

In an embodiment of the first and/or second aspect of the present invention and particularly in an embodiment of the NR-CZ-NR embodiment Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkynyl and substituted branched alkynyl.

In an embodiment of the first and/or second aspect of the present invention and particularly in an embodiment of the NR-CZ-NR embodiment Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide. Alternatively, Y can be absent.

In an embodiment of the NR-CZ-NR embodiment R<sup>c</sup> and/or R<sup>d</sup> are independently from each other selected from the group alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl,

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alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl.

In a particularly preferred embodiment of the first and the second aspect of the present invention which is also referred to as the NR embodiment is X is

$$-(CR^aR^b)_n-NR^c-(CR^fR^g)_m-$$

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In an embodiment R<sup>a</sup>, R<sup>b</sup>, R<sup>c</sup>, R<sup>d</sup>, R<sup>e</sup>, R<sup>f</sup> and R<sup>g</sup> are independently from each other selected from the group H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, heteroaryl, substituted heteroaryl.

In an embodiment  $R_5$  is selected from the group comprising H and -C(O)-Q. Preferably  $R_5$  is H.

In a further embodiment m is any integer between 1 and 10. Preferably n is 0.

In a still further embodiment  $R_5$  is selected from the group comprising H and -C(O)-Q, whereby m is any integer between 1 and 10. Preferably n is 0. In an even more preferred embodiment  $R_5$  is H.

In a preferred embodiment of the NR embodiment X is  $-(CR^aR^b)_n-NR^c-(CR^fR^g)_m$ , and

wherein t is 1. Preferably, Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, and substituted branched alkynyl. Preferably  $R_5$  is selected from the group comprising H and -C(O)-Q and even more preferably  $R_5$  is H. In a still further preferred embodiment n is 0.

In a preferred embodiment of the NR embodiment, wherein X is  $-(CR^aR^b)_n-NR^c-(CR^fR^g)_m$ , and

wherein t is 1m is any integer between 1 and 10, preferably m is any integer between 2 and 10. Preferably, R<sub>5</sub> is selected from the group comprising H and -C(O)-Q, and more preferably R<sub>5</sub> is H. Also preferably Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or is absent.

In a preferred embodiment  $R_5$  is selected from the group comprising H and -C(O)-Q, preferably  $R_5$  is H and even more preferably n is 0.

In a particularly preferred embodiment of the first and the second aspect of the present invention which is also referred to as the NR-Z embodiment X is

-(CR<sup>a</sup>R<sup>b</sup>)<sub>n</sub>-NR<sup>c</sup>-Z-(CR<sup>f</sup>R<sup>g</sup>)<sub>m</sub>- and can be inserted in any orientation into any of the preceding formulae,

and wherein Z is selected from the group comprising C(O), C(S), S(O<sub>2</sub>), C(O)-O, and C(O)-S.

In an embodiment  $R_5$  is selected from the group comprising H and -C(O)-Q, preferably  $R_5$  is H.

In an embodiment n is 0.

In a further embodiment of the NR-Z embodiment X is

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-(CR<sup>a</sup>R<sup>b</sup>)<sub>n</sub>-NR<sup>c</sup>-Z-(CR<sup>f</sup>R<sup>g</sup>)<sub>m</sub>- and can be inserted in any orientation into any of the preceding formulae,

and Z is selected from the group comprising C(O), C(S), S(O<sub>2</sub>), C(O)-O, and C(O)-S, and

wherein preferably t is 1. Preferably Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, and substituted branched alkynyl. More preferably  $R_5$  is selected from the group comprising H and -C(O)-Q and even more preferably  $R_5$  is H. In any of the latter embodiments n is 0.

In a further embodiment of the NR-Z embodiment wherein X is

-(CR<sup>a</sup>R<sup>b</sup>)<sub>n</sub>-NR<sup>c</sup>-Z-(CR<sup>f</sup>R<sup>g</sup>)<sub>m</sub>- and can be inserted in any orientation into any of the preceding formulae,

and Z is selected from the group comprising C(O), C(S), S(O2), C(O)-O, and C(O)-S, and

wherein preferably t is 1, m is any integer between 1 and 10. Preferably,  $R_5$  is selected from the group comprising H and -C(O)-Q, and more preferably  $R_5$  is H. In an embodiment of the latter embodiments Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or wherein Y is absent. Preferably,  $R_5$  is selected from the group comprising H and -C(O)-Q, more preferably  $R_5$  is H. In a particularly preferred embodiment n is 0.

In the embodiment where Y is as defined in the preceding paragraph, m is preferably any integer between 2 and 10. Preferably,  $R_5$  is selected from the group comprising H and -C(O)–Q and more preferably  $R_5$  is H. Even more preferably, in any of these embodiments n is 0.

In a third aspect which is actually an embodiment of the first aspect of the invention, the problem is solved by a compound which has any of the structures according to formulae (XIV), (XVI), (XVII) or (XVIII):

wherein R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> and R<sub>4</sub> are each independently selected from the group comprising H, OR<sub>6</sub>, SR<sub>7</sub>, NR<sub>8</sub>R<sub>9</sub>, halo, alkyl, substituted alkyl, alkylaryl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl;

wherein R<sub>1</sub> and R<sub>2</sub>, R<sub>2</sub> and R<sub>3</sub>, R<sub>3</sub> and R<sub>4</sub>, R<sub>1</sub> and R<sub>3</sub>, R<sub>1</sub> and R<sub>4</sub>, and R<sub>2</sub> and R<sub>4</sub> may be linked so as to form a ring comprising 4 to 12 members, preferably 5 to 10 members, more preferably 5 or 6 or 7 members,

wherein  $Z_1$ ,  $Z_2$ ,  $Z_3$  and  $Z_4$  are each and independently selected from the group comprising – C(O)–, –C(S)–, –C(O)– $NR_{10}$ -, –C(S)– $NR_{11}$ -, –C(N–CN)– $NR_{12}$ -, –S(O)-, – $S(O_2)$ –, – $S(O_2)$ –, – $S(O_2)$ – $NR_{14}$ -, –O–, and –S–, or are each and individually absent;

R<sub>5</sub> is selected from the group comprising H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl,

substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl, substituted alkylheteroaryl and -C(O)-Q;

wherein Q is selected from the group comprising H, NHR<sub>15</sub>, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl, and substituted alkylheteroaryl; and

R<sub>6</sub>, R<sub>7</sub>, R<sub>8</sub>, R<sub>9</sub>, R<sub>10</sub>, R<sub>11</sub>, R<sub>12</sub>, R<sub>13</sub>, R<sub>14</sub> and R<sub>15</sub> are each and independently selected from the group comprising H, alkyl, substituted alkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, alkoxy, substituted alkoxy, aryloxy, substituted aryloxy, alkylamino, substituted alkylamino, arylamino and substituted arylamino;

X is a spacer and is independently selected from the group comprising

-M1-L1-K-L2-M2-,

wherein K is selected from the group comprising

C=T,

O, S, S(O) and  $S(O_2)$ ,

or is absent,

with =T being selected from the group comprising

$$=O$$
,  $=S$ ,  $=N-R^e$ ,  $=N-CN$ ,  $=N-NO_2$  and  $=CH-NO_2$ ,

L1 and L2 are each and independently selected from the group comprising

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O, S and primary amines, more particularly NR<sup>c</sup>, NR<sup>d</sup>; or being individually and independent from each other absent

M1 and M2 are each and independently selected from the group comprising -(CR\*aR\*b)n-,
-(CR\*fR\*g)m-,
cycloalkyl, substituted cycloakyl, heterocyclyl, substituted heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl heteroaryl], or being individually and independent from each other absent,

wherein D is  $C_1$ – $C_6$  alkyl, preferably straight  $C_1$ – $C_6$  alkyl,  $C_1$ – $C_6$  alkenyl, preferably straight  $C_1$ – $C_6$  alkynyl, whereby preferably any of the alkyl, alkenyl and alkynyl may individually and independently comprise from 0 to 3 heteroatoms, and/or whereby preferably any of the alkyl, alkenyl and alkynyl can be individually and independently substituted, more preferably by 1 or 2 substituent(s) preferably each independently selected from H, halo,  $OR_{16}$ , alkyl, and substituted alkyl,

wherein n and m are each and independently selected from each other and are each any integer from 0 to 10,

whereby if n is 2 or more, the group(s) –(CR<sup>a</sup>R<sup>b</sup>)– which is/are repeated, can be the same or different from any of the group(s) –(CR<sup>a</sup>R<sup>b</sup>)–,

whereby any individual group can be linked to any other group or any moiety of the compound through a bond selected from the group comprising single bonds, double bonds and triple bonds,

whereby if m is 2 or more, the group(s) -(CR<sup>f</sup>R<sup>g</sup>)- which is/are repeated, can be the same or different from any of the group(s) -(CR<sup>f</sup>R<sup>g</sup>)-,

whereby any individual group can be linked to any other group or any moiety of the compound through a bond selected from the group comprising single bonds, double bonds and triple bonds,

wherein t is independently selected from n and/or m and is any integer from 0 to 10, whereby if t is 2 or more any of the spacer -M1-L1-K-L2-M2- can be the same or different from any of the spacer(s) X repeated,

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wherein

R<sup>c</sup>, R<sup>d</sup> and R<sup>e</sup> are independently from each other selected from the group H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl; and

R<sup>a</sup>, R<sup>b</sup>, R<sup>f</sup> and R<sup>g</sup> are independently from each other selected from the group H, OR<sub>17</sub>, SR<sub>18</sub>, NR<sub>19</sub>R<sub>20</sub>, halo, alkyl, substituted alkyl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl; or may be independently from each other absent, and

wherein E is  $C_1$ – $C_6$  alkyl, preferably straight  $C_1$ – $C_6$  alkyl,  $C_1$ – $C_6$  alkenyl, preferably straight  $C_1$ – $C_6$  alkenyl,  $C_1$ – $C_6$  alkynyl, preferably straight  $C_1$ – $C_6$  alkynyl, whereby preferably any of the alkyl, alkenyl and alkynyl may comprise individually and independently from 0 to 3 heteroatoms, and/or whereby preferably any of the alkyl, alkenyl and alkynyl can be individually and independently substituted by preferably 1 or 2 substituent(s) each preferably independently selected from the group comprising H, halo,  $OR_{21}$ , alkyl, and substituted alkyl.

R<sub>16</sub>, R<sub>17</sub>, R<sub>18</sub>, R<sub>19</sub>, R<sub>20</sub> and R<sub>21</sub> are each and independently selected from the group comprising H, alkyl, substituted alkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, alkoxy, substituted alkoxy, aryloxy, substituted aryloxy, alkylamino, substituted alkylamino, arylamino and substituted arylamino;

wherein Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkynyl, substituted branched alkynyl, cycloalkyl, substituted cycloalkyl, cycloalkyl, substituted cycloalkenyl, heterocyclyl, substituted

heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl,

or wherein Y is absent.

In an embodiment Y is different from a peptide.

In an embodiment of the first and the third aspect of the present invention the moiety A and phenol moiety, respectively forms a cyclic structure with the spacer X and/or Y.

In an embodiment of the first and the third aspect of the present invention the compound is

$$\begin{array}{c} R_{1}-Z_{1} \\ R_{5}O \\ R_{3}-Z_{3} \end{array}, \quad \begin{array}{c} R_{1}-Z_{1} \\ R_{5}O \\ R_{3}-Z_{3} \end{array}, \quad \begin{array}{c} XVI \\ R_{5}O \\ R_{3}-Z_{3} \end{array}, \quad \begin{array}{c} XVI \\ R_{5}O \\ R_{3}-Z_{3} \end{array}, \quad \begin{array}{c} XVI \\ R_{1}-Z_{1} \\ R_{2}-Z_{2} \\ R_{1}-Z_{1} \\ R_{5}O \end{array}$$

or

In a further embodiment of the first and the third aspect of the present invention the compound is selected from the group comprising

In an embodiment of the first and the third aspect of the present invention K is C=T.

In a further embodiment of the first and the third aspect of the present invention T is selected from the group comprising O and S.

In a preferred embodiment of the first and the third aspect of the present invention T is O.

In an alternative preferred embodiment of the first and the third aspect of the present invention T is S.

In a further alternative embodiment of the first and the third aspect of the present invention T is selected from the group comprising N-CN, N-NO<sub>2</sub>, CH-NO<sub>2</sub> and N-R<sup>e</sup>.

In an embodiment of the first and the third aspect of the present invention, more particularly the embodiment where T is either O or S, L1 and L2 are each and independently a primary amine, preferably NR<sup>c</sup> and/or NR<sup>d</sup>.

In an embodiment of the first and the third aspect of the present invention n = 0 and m is any integer from 0 to 10.

In an embodiment of the first and the third aspect of the present invention R<sub>1</sub> and/or R<sub>3</sub> are selected from the group comprising halo, alkyl, substituted alkyl, heterocyclyl, substituted heterocyclyl, heterocy

In an embodiment of the first and the third aspect of the present invention R<sub>5</sub> is selected from the group comprising H and -C(O)-Q. In a preferred embodiment Q is selected from alkylheterocyclyl and substituted alkylheterocyclyl. In an even more preferred embodiment Q is selected from the group comprising N-acylated morpholino-, N-acylated piperazino- and N-acyl-derivatives.

In an embodiment of the first and the third aspect of the present invention  $R_6$  is alkyl or substituted alkyl.

In an embodiment of the first and the third aspect of the present invention R<sub>8</sub> and R<sub>9</sub> are individually and separately selected from the group comprising H, alkyl and substituted alkyl.

In an embodiment of the first and the third aspect of the present invention n and m are individually and independently any integer from 1 to 3.

In an alternative embodiment of the first and the third aspect of the present invention n is any integer from 0 to 3 and is preferably 0 or 1.

In a further alternative embodiment of the first and the third aspect of the present invention n and m are both 0.

In an embodiment of the first and the third aspect of the present invention t is 1 or 2.

In another embodiment of the first and the third aspect of the present invention R<sup>c</sup> and/or R<sup>d</sup> are each and independently from each other selected from the group comprising alkyl,

substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl.

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In still another embodiment of the first and the third aspect of the present invention  $R^a$ ,  $R^b$ ,  $R^f$  and  $R^g$  are each individually and independently from each other selected from the group comprising H,  $OR_{17}$ ,  $SR_{18}$ ,  $NR_{19}R_{20}$ , halo, alkyl and substituted alkyl.

In a preferred embodiment of the first and the third aspect of the present invention Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkylnyl and substituted branched alkynyl.

In an alternate preferred embodiment of the first and the third aspect of the present invention Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or is absent.

In a particularly preferred embodiment of the first and the third aspect of the present invention which is also referred to as the NR-CZ-NR embodiment X is

$$-\!(CR^aR^b)_n\!-\!NR^c\!-\!CZ\!-\!NR^d\!-\!(CR^f\!R^g)_m\!-\!$$

and Z is preferably selected from the group comprising O, S, N-CN, N-NO2 and CH-NO2.

In an embodiment of the NR-CZ-NR embodiment m is any integer from 1 to 10.

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In an embodiment of the NR-CZ-NR embodiment  $R_5$  is selected from the group comprising H and -C(O)-Q, preferably m is any integer from 1 to 10.

In an embodiment of the NR-CZ-NR embodiment wherein R<sub>5</sub> is H.

In an embodiment of the NR-CZ-NR embodiment n is 0, preferably R<sub>5</sub> being selected from the group comprising H and -C(O)-Q, more preferably m being any integer from 1 to 10. In an alternative embodiment n is any integer from 1 to 10.

In an embodiment of the NR-CZ-NR embodiment t is 1.

In an embodiment of the first and/or third aspect of the present invention and particularly in an embodiment of the NR-CZ-NR embodiment Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, branched alkynyl and substituted branched alkynyl.

In an embodiment of the first and/or third aspect of the present invention and particularly in an embodiment of the NR-CZ-NR embodiment Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide. Alternatively, Y can be absent.

In an embodiment of the NR-CZ-NR embodiment R<sup>c</sup> and/or R<sup>d</sup> are independently from each other selected from the group alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted alkylcycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, alkylheterocyclyl, substituted alkylheterocyclyl, heteroaryl, substituted heteroaryl, alkylheteroaryl and substituted alkylheteroaryl.

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In a particularly preferred embodiment of the first and the third aspect of the present invention which is also referred to as the NR embodiment is X is

$$-(CR^aR^b)_n-NR^c-(CR^fR^g)_m-$$

In an embodiment R<sup>a</sup>, R<sup>b</sup>, R<sup>c</sup>, R<sup>d</sup>, R<sup>e</sup>, R<sup>f</sup> and R<sup>g</sup> are independently from each other selected from the group H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, aryl, substituted aryl, alkylaryl, substituted alkylaryl, heterocyclyl, substituted heterocyclyl, heteroaryl, substituted heteroaryl.

In an embodiment  $R_5$  is selected from the group comprising H and -C(O)-Q. Preferably  $R_5$  is H.

In a further embodiment m is any integer between 1 and 10. Preferably n is 0.

In a still further embodiment  $R_5$  is selected from the group comprising H and -C(O)-Q, whereby m is any integer between 1 and 10. Preferably n is 0. In an even more preferred embodiment  $R_5$  is H.

In a preferred embodiment of the NR embodiment X is  $-(CR^aR^b)_n-NR^c-(CR^fR^g)_m$ , and

wherein t is 1. Preferably, Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, and substituted branched alkynyl. Preferably R<sub>5</sub> is selected from the group comprising H and -C(O)-Q and even more preferably R<sub>5</sub> is H. In a still further preferred embodiment n is 0.

In a preferred embodiment of the NR embodiment, wherein X is  $-(CR^aR^b)_n-NR^c-(CR^fR^g)_m$ , and

wherein t is 1m is any integer between 1 and 10, preferably m is any integer between 2 and 10. Preferably, R<sub>5</sub> is selected from the group comprising H and -C(O)-Q, and more preferably R<sub>5</sub> is H. Also preferably Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, poly-substituted poly-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or is absent.

In a preferred embodiment  $R_5$  is selected from the group comprising H and -C(O)-Q, preferably  $R_5$  is H and even more preferably n is 0.

In a particularly preferred embodiment of the first and the third aspect of the present invention which is also referred to as the NR-Z embodiment X is

-(CR<sup>a</sup>R<sup>b</sup>)<sub>n</sub>-NR<sup>c</sup>-Z-(CR<sup>f</sup>R<sup>g</sup>)<sub>m</sub>- and can be inserted in any orientation into any of the preceding formulae,

and wherein Z is selected from the group comprising C(O), C(S), S(O<sub>2</sub>), C(O)-O, and C(O)-S.

In an embodiment  $R_5$  is selected from the group comprising H and -C(O)-Q, preferably  $R_5$  is H.

In an embodiment n is 0.

In a further embodiment of the NR-Z embodiment X is

-(CR<sup>a</sup>R<sup>b</sup>)<sub>n</sub>-NR<sup>c</sup>-Z-(CR<sup>f</sup>R<sup>g</sup>)<sub>m</sub>- and can be inserted in any orientation into any of the preceding formulae,

and Z is selected from the group comprising C(O), C(S), S(O2), C(O)-O, and C(O)-S, and

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wherein preferably t is 1. Preferably Y is selected from the group comprising alkyl, substituted alkyl, straight alkyl, substituted straight alkyl, branched alkyl, substituted branched alkyl, straight alkenyl, substituted straight alkenyl, branched alkenyl, substituted branched alkenyl, straight alkynyl, substituted straight alkynyl, and substituted branched alkynyl. More preferably  $R_5$  is selected from the group comprising H and -C(O)—Q and even more preferably  $R_5$  is H. In any of the latter embodiments n is 0.

In a further embodiment of the NR-Z embodiment wherein X is

-(CR<sup>a</sup>R<sup>b</sup>)<sub>n</sub>-NR<sup>c</sup>-Z-(CR<sup>f</sup>R<sup>g</sup>)<sub>m</sub>- and can be inserted in any orientation into any of the preceding formulae,

and Z is selected from the group comprising C(O), C(S), S(O2), C(O)-O, and C(O)-S, and

wherein preferably t is 1, m is any integer between 1 and 10. Preferably,  $R_5$  is selected from the group comprising H and -C(O)-Q, and more preferably  $R_5$  is H. In an embodiment of the latter embodiments Y is selected from the group comprising cycloalkyl, substituted cycloalkyl, cycloalkenyl, substituted cycloalkenyl, heterocyclyl, substituted heterocyclyl, mono-unsaturated heterocyclyl, poly-unsaturated heterocyclyl, mono-substituted poly-unsaturated heterocyclyl, mono-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, poly-substituted mono-unsaturated heterocyclyl, aryl, substituted aryl, heteroaryl and substituted heteroaryl, wherein Y is different from a peptide or wherein Y is absent. Preferably,  $R_5$  is selected from the group comprising H and -C(O)-Q, more preferably  $R_5$  is H. In a particularly preferred embodiment n is 0.

In the embodiment where Y is as defined in the preceding paragraph, m is preferably any integer between 2 and 10. Preferably,  $R_5$  is selected from the group comprising H and -C(O)–Q and more preferably  $R_5$  is H. Even more preferably, in any of these embodiments n is 0.

As used herein, any integer between or any integer from e.g., 0 and 10 or 0 to 10 means 1, 2, 3, 4, 5, 6, 7, 8, 9 and 10.

In an embodiment of any aspect of the present invention Y is different from a peptide. As used herein peptide means a polymer of at least two amino acids which are linked by an amide bond. Any of the amino acids may be a natural or a non natural acid.

In a preferred embodiment of any aspect of the present invention m, n and t are independently selected from each other and are preferably any integer between 0 and 5; more preferably if n is 0, m is different from 0 and if m is 0, n is different from 0.

Also as used herein the term compound(s) according to the present invention means any compound(s) according to any aspect of the present invention. If not indicated to the contrary, any embodiment of the present invention is an embodiment of any aspect of the present invention.

Re is selected from the group comprising H, alkyl, aryl, alkoxy, aryloxy, alkylamino and arylamino.

In an even more preferred embodiment of the inventive compound R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> R<sub>4</sub> and/or R<sub>5</sub> have independently from each other one or more groups of the formula R<sup>f</sup>; whereby R<sup>f</sup> is selected from the group comprising alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl, alkoxy, aryloxy, arylalkoxy, alkoxycarbonyl, aryloxycarbonyl, alkanoyl, aroyl, alkanoyloxy, aroyloxy, carbamoyl, alkanoylamino, aroylamino, alkylthio, arylthio, ureido and amine.

## In a further preferred embodiment

the alkylthio group is derivatized, preferably the sulfur atom of the alkylthio group is oxidized to a sulfoxide or sulfone;

the arylthio group is derivatized, preferably the sulfur atom of the arylthio group is oxidized to a sulfoxide or sulfone,

the ureido group is derivatized, preferably the nitrogen atom of the ureido group is independently mono- or di-substituted, more preferably the substitution is selected from the group comprising alkyl, aryl, heterocyclyl, heteroaryl, alkoxycarbonylamino,

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aryloxycarbonylamino, alkylcarbamoyloxy, arylcarbamoyloxy, alkylsulfonylamino, arylsulfonylamino, alkylaminosulfonyl, and arylaminosulfonyl; and/or

the amino group is derivatized, preferably the nitrogen atom is independently mono- or disubstituted by alkly, aryl, heterocyclyl, heteroalyl, halogen, hydroxy, oxo, carboxy, cyano, nitro, amidino and guanidino.

In a still more preferred embodiment R<sup>f</sup> is further substituted by one ore more groups R<sup>g</sup>, whereby R<sup>g</sup> is selected from the group comprising alkyl, cycloalkyl, aryl, arylalkyl, alkoxy, aryloxy, arylalkoxy, alkanoyl, aroyl, amino, halogen, hydroxy, oxo, carboxy, cyano, nitro, amidino and guanidino.

Particularly preferred compounds according to the present invention are the compounds specified in the following table 1:

	Structure	Chemical name	Formula	Synthesis methods	MolWeight	MS data
-	TX =0	3-[3-(5-Chloro-2-hydroxy-phenyl)- ureido]-propionic acid ethyl ester	C12H15CIN2O4	¥	286.71	286.9
7	h o h	1-(5-Chloro-2-hydroxy-phenyl)-3- pentyl-urea	C12H17CIN2O2	Ą	256.73	256.9
m	TIN TIN TIN TIN TIN TIN TIN TIN TIN TIN	1-Benzyl-3-(5-chloro-2-hydroxy- phenyl)-urea	C14H13CIN2O2	<b>∀</b>	276.72	276.9
4	TIN DIN E	1-(5-Chloro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-urea	C15H15CIN2O2	<b>∀</b>	290.74	290.9
٧٠	12 5 12 5	I-(5-Chloro-2-hydroxy-phenyl)-3- phenethyl-urea	C15H15CIN2O2	∢	290.75	291.2

5 12 22 5 72 75 75	1-(5-Chloro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea	C15H23CIN2O2	Ą	298.81	299.4
IZ O IZ TO	1-tert-Butyl-3-(5-chloro-2- hydroxy-phenyl)-urea	C11H15CIN2O2	∢	242.70	243.0
IN DO	1-(5-Chloro-2-hydroxy-phenyl)-3- cyclohexylmethyl-urea	C14H19CIN2O2	. ∀	282.77	283.1
₹ 5 0 ± 2 0 ± 2 0 ± 2 0 0 ± 2 0 0 0 0 0 0 0	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	C15H12CIF3N2O2	<b>∀</b>	344.72	345.0
12 0 12 0 TO	1-(5-Chloro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-urea	C13H9Cl3N2O2	∢	331.59	331.9

		r		
297.7	331.0	269.1	346.9	. 287.9
297.14	330.69	268.74	346.69	287.70
¥	¥	¥	¥	¥
C13H10CIZNZO2	C14H10CIF3N2O2	C13H17CIN2O2	C14H10CIF3N2O3	C14H10CIN3O2
1-(5-Chloro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- cyclohexyl-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethoxy-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-cyano-phenyl)-urea
5 0 IZ 0	P N O	12 0 12 5	P N OCES	\$ 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
11	12	13	14	51

306.9	276.9	292.9	290.9	. 353.2
306.70	276.72	27.262	290.75	352.77
ď	Ą	Ą	A	٧
C14H11CIN2O4	C14H13CIN2O2	C14H13CIN2O3	C15H15CIN2O2	C16H17CIN2O5
1-Benzo[1,3]dioxol-5-yl-3-(5- chloro-2-hydroxy-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- o-tolyl-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (3-methoxy-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (2,6-dimethyl-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea
		TN TO THE POPULATION OF THE PO	TZ TZ TZ	HO HO OMe
91	17	18.	19	20

313.1	321.4	354.9	263.2	321.9
312.75	320.82	354.79	262.70	321.16
Ą	<b>∀</b>	· •	A	Ą
C17H13CIN2O2	C17H21CIN2O2	C19H15CIN2O3	C13H11CIN2O2	C12H14Cl2N2O4
1-(5-Chloro-2-hydroxy-phenyl)-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(5-chloro-2- hydroxy-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-phenoxy-phenyl)-urea	1-(5-Chloro-2-hydroxy-phenyl)-3- phenyl-urea	3-[3-(3,5-Dichloro-2-hydroxy- phenyl)-ureido]-propionic acid ethyl ester
IN SO	5—————————————————————————————————————	IZ O	1Z 5—0 1Z	HN O
21	22	g	42	22

292.0	312.0	325.9	325.9	334.0
291.17	311.16	325.19	325.19	333.25
А	¥	А	¥	¥
C12H16Cl2N2O2	C14H12Cl2N2O2	CI5H14Cl2N2O2	C15H14Cl2N2O2	C15H22Cl2N2O2
1-(3,5-Dichloro-2-hydroxy- phenyl)-3-pentyl-urea	1-Benzyl-3-(3,5-dichloro-2- hydroxy-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-phenethyl-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-urea
D D D D D D D D D D D D D D D D D D D	E S	TZ O TZ O	D IN DO	2 TZ 0 TZ 0
26	27	78	29	30

				_
277.8	318.1	379.8	366.9	331.9
277.15	317.21	379.16	366.03	331.58
<b>V</b>	Ą	A	¥	Ą
C11H14Cl2N2O2	C14H18Cl2N2O2	C15H11Cl2F3N2O2	C13H8Cl4N2O2	C13H9Cl3N2O2
1-tert-Butyl-3-(3,5-dichloro-2- hydroxy-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-cyclohexylmethyl-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-chloro-phenyl)-urea
		HN O	D TZ O	
31	32	33	34	35

		Т		
365.9	304.0	381.8	322.9	. 341.7
365.13	303.18	381.13	322.15	341.15
∢	¥	Ą	٧	<b>∀</b>
C14H9Cl2F3N2O2	C13H16Cl2N2O2	C14H9Cl2F3N2O3	C14H9Cl2N3O2	C14H10C12N2O4
1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-cyclohexyl-urea	1-(3,5-Dichloro-2-hydroxy-phenyl)-3-(4-trifluoromethoxy-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-phenyl)-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3,5-dichloro-2-hydroxy-phenyl)-urea
A STOCK STOC	Q IZ IZ O	D IN	12 0 12 5	IZ TZ TZ TZ
36	37	38	39	40

41		1-(3,5-Dichloro-2-hydroxy- phenyl)-3-o-tolyl-urea	C14H12Cl2N2O2	¥	311.16	311.8
42	D D D D D D D D D D D D D D D D D D D	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(3-methoxy-phenyl)- urea	C14H12Cl2N2O3	¥	327.16	327.5
43	2 TZ TZ	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(2,6-dimethyl-phenyl)- urea	C15H14Cl2N2O2	∢	325.19	325.6
4	CI CI CING	1-(3,5-Dichloro-2-hydroxy-phenyl)-3-(3,4,5-trimethoxy-phenyl)-urea	C16H17Cl2N2O5	<b>V</b>	387.21	387.6
45	TZ O TZ O	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-naphthalen-1-yl-urea	C17H12Cl2N2O2	∢	347.20	. 347.6

			<del></del>	•	
355.7	389.6	7.75	286.9	. 256.9	276.9
355.26	389.23	297.14	286.71	256.73	276.72
<b>∢</b>	Ą	¥	A	A	¥
C17H20C12N2O2	C19H14Cl2N2O3	C13H10Cl2N2O2	C12H15GIN2O4	C12H17CIN2O2	C14H13CIN2O2
1-Adamantan-1-yl-3-(3,5-dichloro- 2-hydroxy-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-phenoxy-phenyl)- urea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-phenyl-urea	3-[3-(3-Chloro-2-hydroxy-phenyl)- ureido]-propionic acid ethyl ester	1-(3-Chloro-2-hydroxy-phenyl)-3- pentyl-urea	1-Benzyl-3-(3-chloro-2-hydroxy- phenyl)-urea
5 -5 -5	2 IZ 0 IZ 0	5 5 5 7 5	D IN	E S	TIN TO TIN TO TIN
46	47	48	49	20	51

			<del></del>			
290.9	291.2	299.4	243.0	283.1	. 345.0	331.9
290.74	290.75	298.81	242.70	282.77	344.72	331.59
A	∢	¥	Ą	<b>V</b>	¥	¥
C15H15CIN2O2	C15H15CIN2O2	CISH23CIN2O2	CI1H15CIN2O2	C14H19CIN2O2	C15H12CIF3N2O2	C13H9Cl3N2O2
1-(3-Chloro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- phenethyl-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-(3-chloro-2- hydroxy-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- cyclohexylmethyl-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-urea
TZ O	P S S S S S S S S S S S S S S S S S S S	TZ O	12 0 12 0 12 0	IZ TZ TO TZ	D CP.	5 12 5 12 5
52	53	54	55	56	57	28

59	IZ D	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-urea	C13H10Cl2N2O2	ď	297.14	297.7
09	TIN HO TO	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)-urea	C14H10CIF3N2O2	∢	330.69	331.0
61	D IN	1-(3-Chloro-2-hydroxy-phenyl)-3- cyclohexyl-urea	C13H17CIN2O2	A	268.74	269.1
62	IN I	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethoxy-phenyl)-urea	C14H10CIF3N2O3	Ą	346.69	346.9
63	12 0 12 0 12 0	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-cyano-phenyl)-urea	C14H10CIN3O2	<b>A</b> .	287.70	287.9
2	IZ TZ TZ	1-Benzo[1,3]dioxol-5-yl-3-(3- chloro-2-hydroxy-phenyl)-urea	C14H11CIN2O4	¥	306.70	306.9
65	HN HO HIN	1-(3-Chloro-2-hydroxy-phenyl)-3- o-tolyl-urea	C14H13CINZO2	∢	276.72	276.9

292.9	290.9	353.2	313.1	321.4	354.9
292.72	290.75	352.77	312.75	320.82	354.79
∢	A	Ą	. ∢	<b>⋖</b>	<b>V</b>
C14H13CIN2O3	C15H15CIN2O2	C16H17CIN2O5	C17H13CIN2O2	C17H21CIN2O2	C19H15CIN2O3
1-(3-Chloro-2-hydroxy-phenyl)-3- (3-methoxy-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (2,6-dimethyl-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(3-chloro-2- hydroxy-phenyl)-urea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-phenoxy-phenyl)-urea
CI N N N N N N N N N N N N N N N N N N N	E S	CI CI COMe OMe	P IN O	P T N T N T N T N T N T N T N T N T N T	E S
99	1.9	89	89	0/	17

1-(3-Chloro-2-hydroxy-phenyl)-3- C				
	C13H11CIN2O2	¥	262.70	263.2
3-[3-(3-Fluoro-2-hydroxy-phenyl)- c	C12H15FN2O4	¥	270.26	270.6
1-(3-Fluoro-2-hydroxy-phenyl)-3- C pentyl-urea	C12H17FN2O2	<b>∀</b>	240.27	240.5
1-Benzyl-3-(3-fluoro-2-hydroxy-phenyl)-urea	C14H13FN2O2	<b>V</b>	260.26	260.8
1-(3-Fluoro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-urea	C15H15FN2O2	∢	274.29	274.9
1-(3-Fluoro-2-hydroxy-phenyl)-3- phenethyl-urea	C15H15FN2O2	¥	274.29	274.6
1-(3-Fluoro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea	C15H23FN2O2	<b>.</b>	282.35	282.9

226.5	266.7	328.4	315.5	281.1	314.6
226.25	266.31	328.26	315.13	280.68	314.24
A	∢	Ą	<b>4</b>	¥	A
C11H15FN2O2	C14H19FN2O2	C15H12F4N2O2	C13H9C12FN2O2	C13H10CIFN2O2	C14H10F4N2O2
1-tert-Butyl-3-(3-fluoro-2- hydroxy-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- cyclohexylmethyl-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)-urea
JIZ =0	TZ =0	P CFs	N N N N N N N N N N N N N N N N N N N	HZ HZ	HO H
79	08	18	83	83	\$

		Υ			
336.6	296.6	304.6	338.6	246.5	335.9
336.31	296.3	304.36	338.33	246.24	335.19
A	Ą	<b>⋖</b>	₹	A	¥
C16H17FN2O5	C17H13FN2O2	C17H21FN2O2	C19H15FN2O3	C13H11FN2O2	C13H16C12N2O4
1-(3-Fluoro-2-hydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(3-fluoro-2- hydroxy-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-phenoxy-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- phenyl-urea	3-[3-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-ureido]-propionic acid ethyl ester
F OMe OMe OMe	IZ O IZ	₹ ₹ ₹	₹	TZ TO TZ To	
22	93	*	95	%	16

			<del></del>	
305.9	325.5	339.9	339.4	347.4
305.20	325.19	339.22	339.22	347.28
¥	¥	ď	<b>V</b>	A
C13H18Cl2N2O2	C15H14Cl2N2O2	C16H16Cl2N2O2	C16H16Cl2N2O2	C16H24Cl2N2O2
1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-pentyl-urea	1-Benzyl-3-(3,5-dichloro-2- hydroxy-4-methyl-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(2-methyl- benzyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-phenethyl-urea	1-(3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-3-(1,1,3,3-terramethyl-butyl)-urea
N O	TZ O TZ	TZ TO TZ	TZ TS	TZ O TZ
86	66	100	101	102

			<del></del>	
291.2	332.1	393.8	380.2	. 345.9
291.18	331.24	393.19	380.06	345.61
A	Ą	∢	<b>∢</b>	A
C12H16Cl2N2O2	C15H20Cl2N2O2	C16H13Cl2F3N2O2	C14H10Cl4N2O2	C14H11Cl3N2O2
1-tert-Butyl-3-(3,5-dichloro-2- hydroxy-4-methyl-phenyl)-urea	1-Cyclohexylmethyl-3-(3,5- dichloro-2-hydroxy-4-methyl- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4- trifluoromethyl-benzyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(3,5-dichloro- phenyl)-urea	1-(4-Chloro-phenyl)-3-(3,5- dichloro-2-hydroxy-4-methyl- phenyl)-urea
	IN IN IN IN IN IN IN IN IN IN	D IN O IN	2 TZ	12 0 IZ 5
103	104	105	106	107

379.9	317.8	395.4	336.4	. 355.2
379.16	317.21	395.16	336.18	355.18
<b>«</b>	¥	∢	<b>∀</b>	<b>4</b>
CISHI ICIZF3N2O2	C14H18Cl2N2O2	C15H11Cl2F3N2O3	C15H11Cl2N3O2	C15H12Cl2N2O4
1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4- trifluoromethyl-phenyl)-urea	1-Cyclohexyl-3-(3,5-dichloro-2- hydroxy-4-methyl-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4- trifluoromethoxy-phenyl)-urea	1-(4-Cyano-phenyl)-3-(3,5- dichloro-2-hydroxy-4-methyl- phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3,5-dichloro-2-hydroxy-4-methyl-phenyl)-urea
TZ O TZ O	IZ O IZ TZ	PA NEW TO	HZ O TO	IZ O TZ
108	109	110	1111	112

325.5	341.4	339.4	401.3	. 361.3
325.19	341.19	339.22	401.24	361.23
Ą	¥	∢	A	Ą
C15H14CI2N2O2	C15H14Cl2N2O3	C16H16Cl2N2O2	C17H18C12N2O5	C18H14Cl2N2O2
1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-0-tolyl-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(3-methoxy- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(2,6-dimethyl- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(3,4,5- trimethoxy-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-naphthalen-1-yl- urea
E S	PO NH OME		CI OMe OMe	TZ O TZ
113	114	115	116	117

369.3	403.3	311.3	349.9	320.0
369.29	403.26	311.17	349.15	319.17
¥	A	A	A	¥
C18H22C12N2O2	C20H16C12N2O3	C14H12Cl2N2O2	C12H14BrFN2O4	C12H16BrFN2O2
1-Adamantan-1-yl-3-(3,5-dichloro- 2-hydroxy-4-methyl-phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4-phenoxy- phenyl)-urea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-phenyl-urea	3-[3-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-ureido]-propionic C12H14BrFN2O4 acid ethyl ester	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-pentyl-urea
TZ 0	5 -5 -5 -5 -5 -5		IZ O D D D D D D D D D	IZ H
118	119	120	121	122

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340.0	353.9	353.9	362.0	305.8
339.16	353.19	353.19	361.25	305.14
¥	¥	Α .	<b>V</b>	¥
C14H12BrFN2O2	C15H14BrFN2O2	C15H14BrFN2O2	C15H22BrFN2O2	C11H14BrFN2O2
1-Benzyl-3-(5-bromo-3-fluoro-2- hydroxy-phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-phenethyl-urea	1-(5-Bromo-3-fiuoro-2-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-(5-bromo-3-fluoro- 2-hydroxy-phenyl)-urea
	TZ O TZ	IZ O	IZ TZ TZ TZ TZ TZ	TZ 50
123	124	125	126	127

346.1	407.8	394.9	359.9	393.9
345.21	407.16	394.02	359.58	393.13
¥	¥	∢	٧	¥
C14H18BrFN2O2	C15H11BrF4N2O2	C13H8BrCl2FN2O2	C13H9BrCIFN2O2	C14H9BrF4N2O2
1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-cyclohexylmethyl-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-chloro-phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea
TZ TO TA	P CPs	Br Cci	HO IN	F A N N N N N N N N N N N N N N N N N N
128	129	130	131	132

				- E
332.0	409.8	350.9	369.7	. 339.8
331.18	409.13	350.14	369.14	339.16
٧	٧	∢	∢	¥
C13H16BrFN2O2	C14H9BrF4N2O3	C14H9BrFN3O2	C14H10BrFN2O4	C14H12BrFN2O2
1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-cyclohexyl-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-trifluoromethoxy- phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(5-bromo-3-fluoro-2-hydroxy-phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-o-tolyl-urea
5—————————————————————————————————————	E N OOF,	TZ O TZ	TZ TZ TZ	
133	134	135	136	137

355.5	353.6	415.6	375.6	383.7
355.16	353.19	415.21	375.19	383.26
А	٧	A	∢	ď
C14H12BrFN2O3	C15H14BrFN2O2	C16H17BrFN2O5	C17H12BrFN2O2	C17H20BrFN2O2
1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-(3-methoxy-phenyl)-	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(2,6-dimethyl-phenyl)- urea	1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-(3,4,5-trimethoxy-phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(5-Bromo-3- fluoro-2-hydroxy-phenyl)-urea
HO H	F	Br OMe	TZ o TZ	FINAL PROPERTY OF THE PROPERTY
138	139	140	141	142

		Т	Υ		
417.6	325.7	288.9	258.9	278.8	292.9
417.23	325.13	288.25	258.26	278.25	292.28
¥	¥	₹	¥	¥	V
C19H14BrFN2O3	C13H10BrFN2O2	C12H14F2N2O4	C12H16F2N2O2	C14H12F2N2O2	C15H14F2N2O2
1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-phenoxy-phenyl)- urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-phenyl-urea	3-[3-(3,5-Difluoro-2-hydroxy-phenyl)-ureido]-propionic acid ethyl ester	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-pentyl-urea	1-Benzyl-3-(3,5-difluoro-2- hydroxy-phenyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea
12 0 12 b		HO H	E IZ	IZ O	IZ O
143	44	145	146	147	148

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292.9	300.5	244.3	284.6	346.5	333.3
292.28	300.34	244.24	284.30	346.25	333.12
A	¥	Ą	А	¥	¥
C15H14F2N2O2	C15H22F2N2O2	C11H14F2N2O2	C14H18F2N2O2	C15H11F5N2O2	C13H8CI2F2N2O2
1-(3,5-Difluoro-2-hydroxy- phenyl)-3-phenethyl-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-urea	1-tert-Butyl-3-(3,5-difluoro-2- hydroxy-phenyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-cyclohexylmethyl-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea
E P	HO HO HO	F OH H H	F OH N N	P N N OF 3	TIN TO TI
149	150	151	152	153	154

		<del></del>				···
298.9	332.7	270.7	348.6	289.5	308.5	278.6
298.67	332.23	270.28	348.22	289.24	308.24	278.25
A	Ą	A	<b>V</b>	Ą	A	А
C13H9CIF2N2O2	C14H9F5N2O2	C13H16F2N2O2	C14H9F2F3N2O3	C14H9F2N3O2	C14H10F2N2O4	C14H12F2N2O2
1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(4-chloro-phenyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea	1-(3,5-Difluoro-2-hydroxÿ- phenyl)-3-cyclohexyl-urea	1-(3,5-Difluoro-2-hydroxy-phenyl)-3-(4-trifluoromethoxy-phenyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3,5- difluoro-2-hydroxy-phenyl)-urea	1-(3,5-Difluoro-2-hydroxy- phenyl)-3-o-tolyl-urea
TIX O TIX	TZ O HZ	#Z_0	H N N N N N N N N N N N N N N N N N N N	IZ IZ IZ IZ	\$ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\	EZ E
155	156	157	158	159	991	161

8→	IZ	1-(3,5-Difluoro-2-hydroxy-		•		
		phenyl)-3-(3-methoxy-phenyl)- urea	C14H12F2N2O3	∢	294.25	294.5
F S S S S S S S S S S S S S S S S S S S		1-(3,5-Difluoro-2-hydroxy-phenyl)-3-(2,6-dimethyl-phenyl)-urea	C15H14F2N2O2	Ą	292.28	292.6
TZ TZ TZ	OMe	1-(3,5-Difluoro-2-hydroxy-phenyl)-3-(3,4,5-trimethoxy-phenyl)-urea	C16H17F2N2O5	∢	354.31	354.6
P P P P P P P P P P P P P P P P P P P		1-(3,5-Difluoro-2-hydroxy- phenyl)-3-naphthalen-1-yl-urea	C17H12F2N2O2	. ∢	314.29	314.6
£	- <del>Į</del>	1-Adamantan-1-yl-3-(3,5-difluoro- 2-hydroxy-phenyl)-urea	C17H20F2N2O2	∢	322.35	322.7
TZ TZ TZ		1-(3,5-Difluoro-2-hydroxy-phenyl)-3-(4-phenoxy-phenyl)- urea	C19H14F2N2O3	Ψ .	356.32	356.6

264.7	331.1	301.2	321.0	. 335.1
264.23	330.76	300.78	320.77	334.80
Ą	Ą	A	А	₹
C13H10F2N2O2	C14H19CIN2O5	C14H21CIN2O3	C16H17CIN2O3	C17H19CIN2O3
1-(3,5-Difluoro-2-hydroxy- phenyl)-3-phenyl-urea	3-{3-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-ureido}-propionic acid ethyl ester	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-pentyl-urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-pentyl- urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(2- methyl-benzyl)-urea
P N N N N N N N N N N N N N N N N N N N	N HO HO	N O HO	HO HO TO	IN HO TO
168	169	170	171	172

335.3	343.7	287.6	327.5	389.4
334.80	342.86	286.75	326.82	388.77
¥	A	A		А
C17H19CIN2O3	C17HZ7Cl2N2O2	C13H19CIN2O3	C16H23CIN2O3	C17H16CIF3N2O3
1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3- phenethyl-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-[5-chloro-2- hydroxy-3-(1-hydroxy-ethyl)- phenyl]-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-cyclohexylmethyl-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-benzyl)-urea
12 5 5	P 0 1N 0 1	HO HO HO	£ 5 5	HO HO NO
173	174	175	176	17.1

376.2	341.6	375.0	313.0	. 391.2
375.63	341.19	374.74	312.79	390.74
4	¥	A		¥
C15H13Cl3N2O3	C15H14Cl2N2O3	C16H14CIF3N2O3	C15H21CIN2O3	C16H14ClF3N2O4
1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(4- chloro-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(4- chloro-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-cyclohexyl-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethoxy-phenyl)-urea
HO HO HO TO	P P P P P P P P P P P P P P P P P P P	N N N N N N N N N N N N N N N N N N N	TZ O TZ Ö Ö	OCF <sub>2</sub>
178	179	180	181	182

332.0	351.1	321.0	337.1	. 335.2
331.75	350.75	320.77	336.77	334.80
A	¥	Ą	A	¥
C16H14CIN3O3	C16H15CIN2O5	C16H17CIN2O3	C16H17CINZO4	C17H19CIN2O3
1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-[5-chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-o-tolylurea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(3-methoxy-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(2,6- dimethyl-phenyl)-urea
OH O	OH OH OH OC	IN O HO	OH OH OHO	IN IO
183	184	185	186	187

	,	T		
397.2	357.1	365.1	399.0	307.0
396.82	356.80	364.87	398.84	306.74
<b>∀</b>	A	. ₹	¥	A
C18H21CIN2O6	C19H17CIN2O3	C19H25CIN2O3	C21H19CIN2O4	C15H15GIN2O3
1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(3,4,5-trimethoxy-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-[5-chloro-2- hydroxy-3-(1-hydroxy-ethyl)- phenyl]-urea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(4-phenyl)-urea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-phenyl- urea
OH OH OM9	P P P P P P P P P P P P P P P P P P P	40 40 12 12 10 10	HO HO TO	TIN TO
188	189	190	191	192

272.9	293.1	306.9	307.1	315.0
97.272	292.78	306.81	306.81	314.87
I	I	Ι.	I	
C12H17GIN2OS	C14H13CINZOS	C15H15CIN2OS	C15H15GIN2OS	C15H23CIN2OS
1-(5-Chloro-2-hydroxy-phenyl)-3- pentyl-thiourea	1-Benzyl-3-(5-chloro-2-hydroxy- phenyl)-thiourea	1-(5-Chloro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-thiourea	1-(5-Chloro-2-hydroxy-phenyl)-3- phenethyl-thiourea	1-(5-Chloro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea
IN I	E S	EZ S	H S S S S S S S S S S S S S S S S S S S	TX SO TX
193	194	195	196	197

OH H H S 1-tert-Butyl-3-(5-chloro-2-hydroxy-phenyl)-thiourea	1-tert-Butyl-3-(5-chlo hydroxy-phenyl)-thio	ro-2- urea	C11H15CIN2OS	I	258.77	258.9
IN I		1-(5-Chloro-2-hydroxy-phenyl)-3- isopropyl-thiourea	C10H13CINZOS	н	244.74	245.0
₹————————————————————————————————————		1-(5-Chloro-2-hydroxy-phenyl)-3- cyclohexylmethyl-thiourea	C14H19CIN2OS	· H	298.83	299.1
	ည်	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	C15H12CIF3N2OS	-	360.78	361.1
12 0 12 0 0 0 0 0 0	5	1-(5-Chloro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-thiourea	C13H9Cl3N2OS	H	347.65	347.9

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	5 12 5 5	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-thiourea	C13H10Cl2N2OS	<b>Jens</b>	313.20	313.5	
5 8	N S S S S S S S S S S S S S S S S S S S	1-(5-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	C14H10ClF3N2OS	н	346.76	347.0	
<del>5</del> — <u></u>	IZ SO	1-(5-Chloro-2-hydroxy-phenyl)-3- cyclohexyl-thiourea	C13H17CIN2OS	I	284.80	285.0	
	TZ w	1-(5-Chloro-2-hydroxy-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	C14H10CIF3N2OS	I	346.76	347.0	
	TZ SS	1-(5-Chloro-2-hydroxy-phenyl)-3- phenyl-thiourea	C13H11CIN2OS	П	278.76	. 279.0	

307.5	327.4	341.4	341.5	. 349.6
307.24	327.23	341.26	341.26	349.32
I	ы	I	Ι	I
C12H16CI2N2OS	C14H12CI2N2OS	C15H14Cl2N2OS	C15H14CI2N2OS	C15H22CI2N2OS
1-(3,5-Dichloro-2-hydroxy- phenyl)-3-pentyl-thiourea	1-Benzyl-3-(3,5-dichloro-2- hydroxy-phenyl)-thiourea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)- thiourea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-phenethyl-thiourea	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-thiourea
2 IZ o	JZ JZ S	IN SOLUTION STATE OF THE STATE	2 ZZ S	2 IX S
208	209	210	211	212

		1-tert-Butyl-3-(3,5-dichloro-2- hydroxy-phenyl)-thiourea	C11H14Cl2N2OS	н	293.21	293.6
5	IZ IZ	1-(5-Chloro-2-hydroxy-phenyl)-3- isopropyl-thiourea	C10H12CIZN2OS	1	279.19	279.5
5 5	IZ SO	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea	C14H18Cl2N2OS	·	333.28	333.5
5—5	IZ 00	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-thiourea	C15H11Cl2F3N2OS	Ι	395.23	395.5
5	TX TX	1-(3,5-Dichloro-2-hydroxy-phenyl)-3-(3,5-dichloro-phenyl)-thiourea	C13H8Cl4N2OS	H	382.09	382.3

\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	IZ	1-(3,5-Dichloro-2-hydroxy-	3 Contraction	-	245.65	245.0
	ō	pheny1/-5-(4-cmoto-pheny1/- thiourea	SOZNEDSICIO	4	245.00	
TZ or TZ	် ဦ	1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiourea	C14H9Cl2F3N2OS	I	381.2	381.6
D IN		1-(3,5-Dichloro-2-hydroxy- phenyl)-3-cyclohexyl-thiourea	C13H16Cl2N2OS	· I	319.25	319.6
P P P P P P P P P P P P P P P P P P P		1-(3,5-Dichloro-2-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea	C14H9Cl2F3N2OS	I	381.20	381.4
TX TX		1-(3,5-Dichloro-2-hydroxy- phenyl)-3-phenyl-thiourea	C13H10Cl2N2OS	I	313.20	. 313.5
D IN S IN S	/	1-(3-Chloro-2-hydroxy-phenyl)-3- pentyl-thiourea	C12H17CIN2OS	I	272.79	273.2

293.1	307.0	307.1	315.2	259.0	. 244.9	299.3
292.78	306.81	306.81	314.87	258.77	244.74	298.83
I	I	I	Ι.	I	I	I
C14H13CIN2OS	C15H15CIN2OS	C15H15CIN2OS	C15H23CIN2OS	C11H15CIN2OS	C10H13CIN2OS	C14H19CIN2OS
1-Benzyl-3-(3-chloro-2-hydroxy- phenyl)-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- phenethyl-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	1-tert-Butyl-3-(3-Chloro-2- hydroxy-phenyl)-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- isopropyl-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- cyclohexylmethyl-thiourea
IZ S	CO H H H N	D H H H N H N H N H N H N H N H N H N H	H H S	HO HO S	CC	E E S
224	225	226	227	228	229	230

361.1	348.0	313.5	347.2	285.1	347.2	279.0
360.78	347.65	313.20	346.76	284.8	346.76	278.76
Н	I	I	I	I	I	-
C15H12CIF3N2OS	C13H9Cl3N2OS	C13H10Cl2N2OS	C14H10CIF3N2OS	C13H17CINZOS	C14H10CIF3N2OS	CI3HIICINZOS
1-(3-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- cyclohexyl-thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	1-(3-Chloro-2-hydroxy-phenyl)-3- phenyl-thiourea
P H N N N N N N N N N N N N N N N N N N	CI COH CI COL	CI C	CI N H N N CF3	OH N N N N N N N N N N N N N N N N N N N	G CF3	N H H H H H H H H H H H H H H H H H H H
231	232	233	234	235	236	237

		Γ		<del></del>	-	
256.8	276.7	290.5	290.5	298.7	. 242.8	228.5
256.34	276.33	290.36	290.36	298.42	242.31	228.29
Ι	I	I	·	· I	I	I
C12H17FN2OS	C14H13FN2OS	C15H15FN2OS	C15H15FN2OS	C15H23FN2OS	CIIHISFNZOS	C10H13FN2OS
1-(3-Fluoro-2-hydroxy-phenyl)-3- pentyl-thiourea	1-Benzyl-3-(3-fluoro-2-hydroxy- phenyl)-thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (2-methyl-benzyl)-thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- phenethyl-thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	1-tert-Butyl-3-(3-fluoro-2- hydroxy-phenyl)-thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- isopropyl-thiourea
IN I	PHO H	F OH H H	F OH N N	F OH N H	HO IN S	4
238	239	240	241	242	243	244

		Γ			
282.7	344.7	331.5	297.1	330.6	. 268.6
282.38	344.33	331.19	296.75	330.30	268.35
·I	Н		<b>.</b>	-	Н
C14H19FN2OS	C15H12F4N2OS	C13H9CIZFN2OS	C13H10CIFN2OS	C14H10F4N2OS	C13H17FN2OS
1-(3-Fluoro-2-hydroxy-phenyl)-3- cyclohexylmethyl-thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-chloro-phenyl)-thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- cyclohexyl-thiourea
F OH N N	OH N N CPs	THE STATE OF THE S	N N N N N N N N N N N N N N N N N N N	P. H. N. H.	E S
245	246	247	248	249	250

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330.5	262.5	321.8	341.5	355.6	355.6
330.30	262.30	321.27	341.26	355.28	355.28
Н	I	Ι	·	I	н .
C14H10F4N2OS	C13H11FN2OS	C13H18CI2N2OS	C15H14Cl2N2OS	C16H16Cl2N2OS	C16H16CIZNZOS
1-(3-Fluoro-2-hydroxy-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	1-(3-Fluoro-2-hydroxy-phenyl)-3- phenyl-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-pentyl-thiourea	1-Benzyl-3-(3,5-dichloro-2- hydroxy-4-methyl-phenyl)- thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(2-methyl- benzyl)-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-phenethyl- thiourea
F OH N OF S	F OH N N	CI OH N N N	Q OH NH NH S	D TN S	TZ S
251	252	253	254	255	256

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363.6	307.5	293.6	347.5	409.5
363.35	307.24	293.21	347.30	409.25
Н	П	H		H
C16H24CIZN2OS	C12H16C12N2OS	C11H14Cl2N2OS	C15H20Cl2N2OS	C16H13Cl2F3N2OS
1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(1,1,3,3- tetramethyl-butyl)-thiourea	1-tert-Butyl-3-(3,5-dichloro-2- hydroxy-4-methyl-phenyl)- thiourea	1-(5-Chloro-2-hydroxy-4-methyl- phenyl)-3-isopropyl-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3- cyclohexylmethyl-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4- trifluoromethyl-benzyl)-thiourea
CI C	HO HO IS	CI OH N N N	CI NH NH NH SI NH SI NH	CI OH N CF3
257	258	259	260	261

396.3	361.9	395.7	333.8	. 395.8
396.12	361.67	395.23	333.28	395.23
ı	П		I	-
C14H10C14N2OS	C14H11Cl3N2OS	C15H11Cl2F3N2OS	C14H18CI2N2OS	C15H11Cl2F3N2OS
1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(3,5-dichloro- phenyl)-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4-chloro- phenyl)-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(4- trifluoromethyl-phenyl)-thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-cyclohexyl- thiourea	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-(2- trifluoromethyl-phenyl)-thiourea
	S S S S S S S S S S S S S S S S S S S	CAN THE SECOND S	D TN S TN S	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
262	263	264	265	266

267	PA S	1-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-3-phenyl-thiourea	C14H12Cl2N2OS	H	327.23	327.7
268	N N N N N N N N N N N N N N N N N N N	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-pentyl-thiourea	C12H16BrFN2OS	Ι	335.24	335.8
269	TN S TN S	1-Benzyl-3-(5-bromo-3-fluoro-2- hydroxy-phenyl)-thiourea	C14H12BrFN2OS	I	355.23	355.4
270	TN N N N N N N N N N N N N N N N N N N	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)- thiourea	C15H14BrFN2OS	I	369.25	369.5
271	HO H	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-phenethyl-thiourea	C15H14BrFN2OS	н	369.25	369.5

377.5	321.5	307.4	361.5	423.5
377.32	321.21	307.19	361.28	423.23
I	н	<b>H</b>	· <b>⊢</b>	I
C15HZ2BrFN2OS	C11H14BrFN2OS	C10H12BrFN2OS	C14H18BrFN2OS	C15H11BrF4N2OS
1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-thiourea	1-tert-Butyl-3-(5-bromo-3-fluoro- 2-hydroxy-phenyl)-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-isopropyl-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-thiourea
E S S S S S S S S S S S S S S S S S S S	IN I	TZ Jā	HN S FE	TH S
272	273	274	275	276

410.5	375.9	409.5	347.6	. 409.5
410.09	375.65	409.20	347.25	409.20
I	I	I	. 1	<b>—</b>
C13H8BrCl2FN2OS	C13H9BrCIFN2OS	C14H9BrF4N2OS	C13H16BrFN2OS	C14H9BrF4N2OS
1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-(3,5-dichloro-phenyl)-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-chloro-phenyl)- thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-3-cyclohexyl-thiourea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea
HN S HN S PA	HA PAGE 18 AND	Property of the state of the st	AN N N N N N N N N N N N N N N N N N N	HN FO FINANCE OF THE PROPERTY
277	278	279	280	281

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341.5	274.8	294.7	308.6	308.6	316.8
341.20	274.33	294.32	308.35	308.35	316.41
Ι	I	I	·	Ι	I
C13H10BrFN2OS	C12H16F2N2OS	C14H12F2N2OS	C15H14F2N2OS	C15H14F2N2OS	C15H22F2N2OS
1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-phenyl-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-pentyl-thiourea	1-Benzyl-3-(3,4-difluoro-2- hydroxy-phenyl)-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)- thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-phenethyl-thiourea	1-(3,4-Difluoro-2-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-thiourea
IN NO TEN	D IN	HN HO LA	F H H S N N N N N N N N N N N N N N N N N	F OH H W	HO IN STANCE OF THE STANCE OF
282	283	284	285	286	287

		T			
260.5	246.5	300.6	362.8	349.7	315.2
260.30	246.28	300.37	362.32	349.18	314.74
H	I	I	<b>PI</b>	Н	<b>F-4</b>
C11H14F2N2OS	C10H12F2N2OS	C14H18F2N2OS	C15H11F5N2OS	C13H8Cl2F2N2OS	C13H9CIF2N2OS
1-tert-Butyl-3-(3,4-Diffuoro-2- hydroxy-phenyl)-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-isopropyl-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- thiourea	1-(3,4-Difluoro-2-hydroxy-phenyl)-3-(4-chloro-phenyl)-thiourea
HO IN	HO HO HA	F OH N N	F CH H KINCTOFS	TY STANDS	HN S HN S S S S S S S S S S S S S S S S
288	289	290	291	292	293

1					
348.8	286.6	348.8	280.5	316.9	337.2
348.29	286.34	348.29	280.29	316.85	336.84
I	П	<b>)</b>	. I	н	1
C14H9F5N2OS	C13H16F2N2OS	C14H9F5N2OS	C13H10F2N2OS	C14H21CIN2O2S	C16H17CIN2O2S
1-(3,4-Difluoro-2-hydroxy-phenyl)-3-(4-trifluoromethyl-phenyl)-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-cyclohexyl-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea	1-(3,4-Difluoro-2-hydroxy- phenyl)-3-phenyl-thiourea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-pentyl-thiourea	1-Benzyl-3-[5-chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-thiourea
F OH W CF3	FN FN S	H CF S	P IX S	45 - 5 12 - 5	2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -
294	295	296	297	298	299

	Structure	Chemical name	Formula	Synthesis methods	MolWeight	MS data
300	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(2-methyl-benzyl)-thiourea	C17H19CINZO2S	I	350.86	351.1
301	HO TIZ	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3- phenethyl-thiourea	C17H19CIN2O2S	I	350.86	351.0
302	TZ SS TS	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(1,1,3,3-teframethyl-butyl)-thiourea	C17H27CIN2O2S	·	358.93	359.2
303	TZ SS TS	1-tert-Butyl-3-[5-chloro-2- hydroxy-3-(1-hydroxy-ethyl)- phenyl]-thiourea	C13H19CINZO2S	I	302.82	303.0
304	HO TIZES	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3- isopropyl-thiourea	C12H17CINZO2S	I	288.79	289.0

		т		-
343.1	405.2	392.0	357.6	391.0
342.88	. 404.83	391.70	357.25	390.81
I	I	· I .	I	I
C16H23CIN2O2S	C17H16CIF3N2O2S	C15H13CI3N2O2S	C15H14Cl2N2O2S	C16H14CIF3N2O2S
1-[5-Chioro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3- cyclohexylmethyl-thiourea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(4- trifluoromethyl-benzyl)-thiourea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(3,5- dichloro-phenyl)-thiourea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-(4- chloro-phenyl)-thiourea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-efhyl)-phenyl]-3-(4-trifluoromethyl-phenyl)-thiourea
P S S S S S S S S S S S S S S S S S S S	HO HO TO	12 % HO - 5	HO HO TO	HO TE S
305	306	307	308	309

329.4	391.0	323.1	342.2	
32,	39	32	35	
328.86	390.81	322.81	341.85	355.88
I	н		Q	D
202S	3N2O2S	7202S	NOS	NOS
C15H21CINZO2S	C16H14CIF3N2O2S	C15H15CIN2O2S	C19H1¢CINOS	C20H18CINOS
1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-cyclohexyl-thiourea	1-[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenyl]-3-(2-trifluoromethyl-phenyl)-thiourea	1-[5-Chloro-2-hydroxy-3-(1- hydroxy-ethyl)-phenyl]-3-phenyl- thiourea	4-Chloro-2-(2-phenylsulfanylbenzylamino)-phenol	4-Chloro-2-(2-p-tolylsulfanyl- benzylamino)-phenol
12 5 12 5 15	12 × 5	TZ SO TZ SO TO	F_0	TZ 5
310	311	312	313	314

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315	5 - v	4-Chloro-2-[2-(4-chloro- phenylsulfanyl)-benzylamino]- phenol	C19H15Cl2NOS	D	376.30	376.8
316	1N 20 20 20 20 20 20 20 20 20 20 20 20 20	4-Chloro-2-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol	C19H15CINZO3S	D	386.85	387.2
317	₽ P	4-Chloro-2-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	C20H18CINO2S	. <b>Q</b>	371.88	372.4
318	12 To 5	4-Chloro-2-[2-(2-chloro- phenylsulfanyl)-benzylamino]- phenol	C19H15Cl2NOS	D	376.30	376.8
319	5 5 5 5	4-Chloro-2-[2-(3-chloro- phenylsulfanyl)-benzylamino]- phenol	C19H15Cl2NOS	D	376.30	376.8

411.2	399.3	393.4	421.7
410.74	398.91	392.90	421.30
Q	Q	Q	Q
C19H14Cl3NOS	C21H19CIN2O2S	C22H17CIN2OS	C19H14CIZN2O3S
4-Chloro-2-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(5-Chloro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	4-Chloro-2-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	4-Chloro-2-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol
2 -2 -2	CH NHAC	IN I	5 2 4 5 
320	321	322	323

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401.2	391.9	408.7	376.7
400.88	391.31	408.30	376.30
Ð	Q	<b>Q</b>	Q
C20H17CIN2O3S	C19H16Cl2N2OS	C19H15CI2NO3S	C19H15Cl2NOS
4-Chloro-2-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-4- chloro-phenol	4-Chloro-2-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol	2,4-Dichloro-6-(2-phenylsulfanyl- benzylamino)-phenol
δ - 5	TN TO TO	P	TZ TZ
324	325	326	327

390.7	411.1	421.8	406.7	411.2
390.33	410.75	421.30	406.33	410.75
Q	D	. О	D	Q
C20H17Cl2NOS	C19H14Cl3NOS	C19H14Cl2N2O3S	C20H17Cl2NO2S	C19H14Cl3NOS
2,4-Dichloro-6-(2-p-tolylsulfanylbenzylamino)-phenol	2,4-Dichloro-6-[2-(4-chloro-phenylsulfanyl)-benzylamino]-phenol	2,4-Dichloro-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	2,4-Dichloro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	2,4-Dichloro-6-[2-(2-chloro- phenylsulfanyl)-benzylamino]- phenol
12 5 5	5 5 5 5	P P P P P P P P P P P P P P P P P P P	P S S S S S S S S S S S S S S S S S S S	2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
328	329	330	331	332

411.2	445.6	433.8	427.8
410.75	445.19	433.36	427.35
Q	D	Q	Q
C19H14Cl3NOS	C19H13Cl4NOS	C21H18Cl2N2O2S	C22H16Cl2N2OS
2,4-Dichloro-6-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2,4-Dichloro-6-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(3,5-Dichloro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2,4-Dichloro-6-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol
5 5 5 5	5 0 12 5 5	C C C C C C C C C C C C C C C C C C C	TN TO TO
333	334	335	336

456.0	435.7	426.0	443.1
455.74	435.33	425.76	442.75
Q		A	Q
C19H13Cl3N2O3S	C20H16Cl2N2O3S	C19H15Cl3N2OS	C19H14Cl3NO3S
2,4-Dichloro-6-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-phenol	2,4-Dichloro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-4,6- dichloro-phenol	2,4-Dichloro-6-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol
0 1 1 1 0	S HZ JO	D D D D D D D D D D D D D D D D D D D	5 5 5 5 5 5
337	338	339	340

342.3	356.3	376.7	387.2	372.2
341.85	355.88	376.30	386.85	371.88
А	Q	O.	Q	Q
C19H16CINOS	C20H18CINOS	C19H15CIZNOS	C19H15CIN2O3S	C20H18CINO2S
2-Chloro-6-(2-phenylsulfanyl- benzylamino)-phenol	2-Chloro-6-(2-p-tolylsulfanyl- benzylamino)-phenol	2-Chloro-6-[2-(4-chloro- phenylsulfanyl)-benzylamino]- phenol	2-Chloro-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	2-Chloro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol
TIN TO	THE STATE OF THE S	P P P P P P P P P P P P P P P P P P P	CI OH NO2	S HA
341	342	343	344	345

376.8	376.8	411.0	399.3	393.4
376.30	376.30	410.74	398.91	392.90
Q	Q	О	Ω	Q
C19H15CIZNOS	C19H15CIZNOS	C19H14CI3NOS	C21H19CINZO2S	C22H17CIN2OS
2-Chloro-6-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Chloro-6-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Chloro-6-[2-(3,4-dichloro- phenylsulfanyl)-benzylamino]- phenol	N-(4-{2-[(3-Chloro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2-Chloro-6-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol
COLUMN SECTION OF THE PROPERTY	CI OH N S	D S S D D	CI CH K	S P P P P P P P P P P P P P P P P P P P
346	347	348	349	350

421.5	[]3	4	3.6
42	401.3	392.4	408.6
421.30	400.88	391.31	408.30
Q	Q	A	A
C19H14Cl2N2O3S	C20H17CINZO3S	C19H16Cl2N2OS	C19H15Cl2NO3S
2-Chloro-6-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2-Chloro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Arnino-2-(4-chloro- phenylsulfanyl)-benzylamino]-6- chloro-phenol	2-Chloro-6-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol
	ON HOW THE WAY TO SEE THE WAY	TN TN TO TO	TIN TO THE TOTAL T
351	352	353	354

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324.6	340.8	360.1	370.8	355.8
325.40	339.43	359.84	370.40	355.43
Q	Q	A	Q	Q
C19H16FNOS	C20H18FNOS	C19H15CIFNOS	C19H15FN2O3S	C20H18FNO2S
2-Fluoro-6-(2-phenylsulfanyl- benzylamino)-phenol	2-Fluoro-6-(2-p-tolylsulfanyl- benzylamino)-phenol	2-Fluoro-6-[2-(4-chloro- phenylsulfanyl)-benzylamino]- phenol	2-Fluoro-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	2-Fluoro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol
TZ S	P S S S S S S S S S S S S S S S S S S S	FN FO	TIN SON	F OH K
355	356	357	358	359

		<del></del>		P
360.2	360.3	394.6	382.9	377.0
359.84	359.84	394.29	382.45	376.45
A	Q	Q	Q	A
C19H15CIFNOS	C19H15CIFNOS	C19H14Cl2FNOS	C21H19FN2O2S	C22H17FN2OS
2-Fluoro-6-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-6-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-6-[2-(3,4-dichloro- phenylsulfanyl)-benzylamino]- phenol	N-(4-{2-[(3-Fluoro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2-Fluoro-6-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol
	HA S	HA H	F OH H	TZ SS
360	361	362	363	364

405.3	384.9	375.1	392.0
404.84	384.42	374.86	391.84
А	Ω	<b>A</b>	Q
C19H14CIFN2O3S	C20H17FN2O3S	C19H16CIFN2OS	C19H15CIFNO3S
2-Fluoro-6-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2-Fluoro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-6-fluoro-phenol	2-Fluoro-6-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol
2	SON TIN	FD S	EN E
365	366	367	368

390.6	404.6	425.2	435.8	420.6
390.33	404.35	424.77	435.32	420.35
А	Q	Q	Q	Α .
C20H17CIZNOS	C21H19CIZNOS	C20H16Cl3NOS	C20H16Cl2N2O3S	C21H19Cl2NO2S
2,4-Dichloro-3-methyl-6-(2-phenylsulfanyl-benzylamino)-phenol	2,4-Dichloro-3-methyl-6-(2-p-tolylsulfanyl-benzylamino)-phenol	2,4-Dichloro-3-methyl-6-[2-(4- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-methyl-6-[2-(4- nitro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-methyl-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol
TX 5	HZ JO	N HO TO	CI OH H S S NO2	- HA HO IO
369	370	371	372	373

		1		
425.1	425.1	459.5	447.8	441.6
424.77	424.77	459.22	447.38	441.37
Q	А	О	Ω	Q
C20H16Cl3NOS	C20H16CI3NOS	C20H15C!4NOS	C22H20Cl2N2O2S	C23H18Cl2N2OS
2,4-Dichloro-3-methyl-6-[2-(2- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-methyl-6-[2-(3- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-methyl-6-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(3,5-Dichloro-2-hydroxy-4-methyl-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2,4-Dichloro-3-methyl-6-[2- (quinolin-7-ylsulfanyl)- benzylamino]-phenol
TN TO	PIN TO	2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -	CI C	
374	375	376	377	378

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470.0	449.6	439.9	457.0
469.77	449.35	439.79	456.77
Q	Q	Q	Q
C20H15Cl3N2O3S	C21H18Cl2N2O3S	C20H17Cl3N2OS	C20H16Cl3NO3S
2,4-Dichloro-3-methyl-6-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-phenol	2,4-Dichloro-3-methyl-6-(5-nitro- 2-p-tolylsulfanyl-benzylamino)- phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-4,6- dichloro-5-methyl-phenol	2,4-Dichloro-3-methyl-6-[2-(4- chloro-benzenesulfonyl)- benzylamino]-phenol
D TN TO			So Si
379	380	381	382

				·
404.7	418.6	439.0	449.8	434.7
404.30	418.33	438.74	449.30	434.33
Q	Д	D	Ω	Q
C19H15BrFNOS	C20H17BrFNOS	C19H14BrCIFNOS	C19H14BrFN2O3S	C20H17B:FNO2S
4-Bromo-2-fluoro-6-(2- phenylsulfanyl-benzylamino)- phenol	4-Bromo-2-fluoro-6-(2-p-tolylsulfanyl-benzylamino)-phenol	4-Bromo-2-[2-(4-chloro-phenylsulfanyl)-benzylamino]-6-fluoro-phenol	4-Bromo-2-fluoro-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	4-Bromo-2-fluoro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol
TZ Š	5_ in	1	E S S S S S S S S S S S S S S S S S S S	F
383	384	385	386	387

484.1	463.7	454.1	471.2
483.74	463.32	453.76	470.74
D	D	Q	Q
C19H13BrCIFN2O3 S	C20H16BrFN2O3S	C19H15BrCIFN2OS	C19H14BrCIFNO3S
4-Bromo-2-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-6-fluoro-phenol	4-Bromo-2-fluoro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-4- bromo-6-fluoro-phenol	4-Bromo-2-[2-(4-chloro-benzenesulfonyl)-benzylamino]-6-fluoro-phenol
N N N N N N N N N N N N N N N N N N N	S TZ Tā	F S S S S S S S S S S S S S S S S S S S	E So
393	394	395	396

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343.6	357.8	378.1	388.8	373.7
343.39	357.42	377.83	388.39	373.42
Q	D	. <b>D</b>	Ω	D
C19H15F2NOS	C20H17F2NOS	C19H14CIF2NOS	C19H14F2N2O3S	C20H17F2NO2S
2,3-Difluoro-6-(2-phenylsulfanyl- benzylamino)-phenol	2,3-Difluoro-6-(2-p-tolylsulfanyl- benzylamino)-phenol	6-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2,3-difluoro-phenol	2,3-Difluoro-6-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol	2,3-Difluoro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol
IZ II	E L	TZ TO	TZ TS LL	TZ B
397	398	399	400	401

378.1	378.2	412.6	400.8	394.9
377.83	377.83	412.28	400.44	394.44
Q	Q	Q	Q	Q
C19H14CIF2NOS	C19H14CIF2NOS	C19H13CIZFZNOS	C21H18F2N2O2S	C22H16F2N2OS
6-[2-(2-Chloro-phenylsufanyl)- benzylamino]-2,3-difluoro-phenol	6-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-2,3-difluoro-phenol	6-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2,3- difluoro-phenol	N-(4-{2-[(3,4-Difluoro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2,3-Difluoro-6-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol
TZ 5	P S	5 5 5 0	P S S NHAC	TZ TO LL
402	403	404	405	406

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423.3	402.8	393.0	392.3
422.83	402.41	392.85	391.84
D	Q	Q	Q
C19H13CIF2N2O3S	C20H16F2N2O3S	C19H15CIF2N2OS	C19H14CIF2NO3S
6-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2,3,-difluoro- phenol	2,3-Difluoro-6-(5-nitro-2-p- tolylsulfanyl-benzylamino)-phenol	6-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-2,3- difluoro-phenol	6-[2-(4-Chloro-benzenesulfonyl)- benzylamino]-2,3-difluoro-phenol
D D D D D D D D D D D D D D D D D D D	P P P P P P P P P P P P P P P P P P P	HO S	TN SCO
407	408	409	410

386.4	. 400.2	420.9	431.3	416.3
385.91	399.93	420.35	430.90	415.93
D	D	Q	A	Q
C21H20CINO2S	C22H22CINO2S	C21H19Cl2NO2S	C21H19CINZO4S	C22H22CINO3S
4-Chloro-2-(1-hydroxy-ethyl)-6- (2-phenylsulfanyl-benzylamino)- phenol	4-Chloro-2-(1-hydroxy-ethyl)-6- (2-p-tolylsulfanyl-benzylamino)- phenol	4-Chloro-2-[2-(4-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	4-Chloro-2-(1-hydroxy-ethyl)-6- [2-(4-nitro-phenylsulfanyl)- benzylamino]-phenol	4-Chloro-2-(1-hydroxy-ethyl)-6- [2-(4-methoxy-phenylsulfanyl)- benzylamino]-phenol
12 5 5 5	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	5 	40 40 10 10 10 10 10 10 10 10 10 10 10 10 10	HO HO IS
411	412	413	414	415

OH O	24 et	4-Chloro-2-[2-(2-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	C21H19CIZNO2S	D	420.35	420.9
OH O	Phe (1-h	4-Chloro-2-[2-(3-chloro- phenylsulfanyl)-benzylamino]-6- (1-hydroxy-ethyl)-phenol	C21H19CIZNO2S	Д	420.35	420.8
OH OH HO HO S C C (1-h)	2-4-0-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1	4-Chloro-2-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-efhyl)-phenol	C21H18Cl3NO2S	. Д	454.80	455.2
OH OH N-[4 (1-h) meth	N-[4 (1-h) meth acetz	N-[4-(2-{[5-Chloro-2-hydroxy-3-(1-hydroxy-ethyl)-phenylamino]-methyl}-phenylsulfanyl)-phenyl]-acetamide	C23H23CIN2O3S	Q	442.96	443.4
OH O	4-Cr [2-(c	4-Chloro-2-(1-hydroxy-ethyl)-6- [2-(quinolin-7-ylsulfanyl)- benzylamino]-phenol	C24H21CINZO2S	Q	436.95	437.3

465.9	445.3	435.6	452.5
465.35	444.93	435.37	452.35
D	D .	Q	Q
C21H18Cl2N2O4S	C22H21CIN2O4S	C21H20Cl2N2O2S	C21H19CI2NO4S
4-Chloro-2-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-6-(1-hydroxy-ethyl)-phenol	4-Chloro-2-(1-hydroxy-ethyl)-6- (5-nitro-2-p-tolylsulfanyl- benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-4- chloro-6-(1-hydroxy-ethyl)-phenol	4-Chloro-2-[2-(4-chloro-benzencsulfonyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol
N HO HO S S S S S	\$	12 5 5 5	F S S
421	422	423	424

337.8	351.8	371.9	382.7	367.9
337.44	351.46	371.88	382.43	367.46
D	Q	D	Q	Q
C20H19NO2S	C21H21NO2S	C20H18CINO2S	C20H18N2O4S	C21H21N03S
2-Hydroxymethyl-6-(2- phenylsulfanyl-benzylamino)- phenol	2-Hydroxymethyl-6-(2-p-tolyisulfanyl-benzylamino)-phenol	2-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-6-hydroxymethyl- phenol	2-Hydroxymethyl-6-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol	2-Hydroxymethyl-6-[2-(4- methoxy-phenylsulfanyl)- benzylamino]-phenol
#Z # # # # # # # # # # # # # # # # # #	TZ TZ TO	12 5 	F. S.	N HO HO
425	426	427	428	429

430	TIZ B B	2-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-6-hydroxymethyl- phenol	C20H18CINO2S	D	371.88	371.9
431	E E	2-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-6-hydroxymethyl- phenol	C20H18CINO2S	Q.	371.88	371.9
432	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	2-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-6- hydroxymethyl-phenol	C20H17Cl2NO2S	. О	406.33	406.5
433	HO-NHAG	N-(4-{2-[(2-Hydroxy-3-hydroxymethyl-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	C22H22N2O3S	Ω	394.49	349.9
434	TZ TO	2-Hydroxymethyl-6-[2-(quinolin-7-ylsulfanyl)-benzylamino]-phenol	C23H20N2O2S	Д	388.48	388.8

417.2	396.8	387.1	44.0
416.88	396.46	386.90	403.88
A	Q	Ω	Q
C20H17CIN2O4S	C21H20N2O4S	C20H19CIN2O2S	C20H18CINO4S
2-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-6- hydroxymethyl-phenol	2-Hydroxymethyl-6-(5-nitro-2-p-tolyisulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-6- hydroxymethyl-phenol	2-[2-(4-Chloro-benzenesulfonyl)- benzylamino]-6-hydroxymethyl- phenol
2 - S	SON HO HO	ZHN HO .	Sto HO HO
435	436	437	438

390.5	418.7	439.0	449.7	434.6
390.33	418.37	438.79	449.34	434.37
D .	D	D	Ω	Q
C21H19Cl2NOS	C22H21Cl2NOS	C21H18Cl3NOS	C21H18CI2N2O3S	C22H21Cl2NO2S
2,4-Dichloro-3-ethyl-6-(2- phenylsulfanyl-benzylamino)- phenol	2,4-Dichloro-3-ethyl-6-(2-p-tolylsulfanyl-benzylamino)-phenol	2,4-Dichloro-3-cthyl-6-[2-(4- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-ethyl-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	2,4-Dichloro-3-ethyl-6-[2-(4- methoxy-phenylsulfanyl)- benzylamino]-phenol
TZ TO TZ	5 5 5	TZ TO	2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	H D D D D D D D D D D D D D D D D D D D
439	440	441	442	443

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438.9	438.9	473.5	461.6	455.7
438.79	438.79	473.24	461.40	455.39
Q	Q	D	Ω	Q
C21H18Ci3NOS	C21H18Cl3NOS	C21H17CI4NOS	C23H22Cl2N2O2S	C24H20CI2N2OS
2,4-Dichloro-3-ethyl-6-[2-(2- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-cthyl-6-[2-(3- chloro-phenylsulfanyl)- benzylamino]-phenol	2,4-Dichloro-3-ethyl-6-[2-(3,4- dichloro-phenylsulfanyl)- benzylamino]-phenol	N-(4-{2-[(3,5-Dichloro-4-ethyl-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	2,4-Dichloro-3-ethyl-6-[2- (quinolin-7-ylsulfanyl)- benzylamino]-phenol
2 ZZ Z	5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5	2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	C C C NHAC	2 5 5 5
444	445	446	447	448

484.0	463.5	454.1	471.0
483.79	463.37	453.81	470.79
Q	Q	<b>Q</b>	Q
C21H17CI3N2O3S	C22H20Cl2N2O3S	C21H19CI3N2OS	C21H18CI3NO3S
2,4-Dichloro-3-ethyl-6-[2-(4- chloro-phenylsulfanyl)-5-nitro- benzylamino]-phenol	2,4-Dichloro-3-ethyl-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	2-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-4,6-dichloro-5-ethyl-phenol	2,4-Dichloro-3-ethyl-6-[2-(4- chloro-benzenesulfonyl)- benzylamino]-phenol
5 5 5 5	S S S S S S S S S S S S S S S S S S S		20 12 20 20 20
449	450	451	452

351.6	365.8	385.1	396.4	381.6
351.42	365.44	385.86	396.11	381.44
Д	Д	О	Q	D
C20H17NO3S	C21H19NO3S	C20H16CINO3S	C20H16N2O5S	C21H19NO4S
2-Hydroxy-3-(2-phenylsulfanyl- benzylamino)-benzoic acid	2-Hydroxy-3-(2-p-tolylsulfanyl- benzylamino)-benzoic acid	3-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxy-benzoic acid	2-Hydroxy-3-[2-(4-nitro- phenylsulfanyl)-benzylamino]- benzoic acid	2-Hydroxy-3-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-benzoic acid
HOOC NH	HOOC NH	HOOC NAME OF THE PART OF THE P	HOOC NO	HOOC NH S
453	454	455	456	457

	Z		
430.9	410.7	387.2	404.1
430.86	410.44	386.90	403.88
D	D	Q	Q
C20H15CIN2O5S	C21H18N2OSS	C20H19CIN2O2S	C20H16CINO5S
3-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2-hydroxy- benzoic acid	2-Hydroxy-3-(5-nitro-2-p-tolylsulfanyl-benzylamino)-benzoic acid	2-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-6-hydroxymethyl-phenol	3-[2-(4-Chloro-benzenesulfonyl)-benzylamino]-2-hydroxy-benzoic acid
HOOC HOOC HOOC HOOC HOOC HOOC HOOC HOOC	HOOOH STATE OF THE PARTY OF THE	HZ HOOOC HZ	HOOOC N N N N N N N N N N N N N N N N N N
463	464	465	466

370.8	384.9	405.0	415.8	400.9
370.40	384.43	404.84	415.40	400.43
D	Q	D	Q	Q
C19H15FN2O3S	C20H17FN2O3S	C19H14CIFN2O3S	C19H14FN3O5S	C20H17FN2O4S
2-Fluoro-4-nitro-6-(2- phenylsulfanyl-benzylamino)- phenol	2-Fluoro-4-nitro-6-(2-p-tolylsulfanyl-benzylamino)-phenol	2-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-6-fluoro-4-nitro- phenol	2-Fluoro-4-nitro-6-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol	2-Fluoro-6-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-4-nitro-phenol
TZ SON	E S	F - 00	TZ SON	NO <sub>2</sub> S S S S S S S S S S S S S S S S S S S
467	468	469	470	471

		<del>_</del>		1
405.0	405.0	439.9	427.9	421.6
404.84	404.84	439.29	427.45	421.45
Д	Д	Q	Q	Q
C19H14CIFN2O3S	C19H14CIFN2O3S	C19H13Cl2FN2O3S	C21H18FN3O4S	C22H16FN3O3S
2-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-6-fluoro-4-mitro- phenol	2-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-6-fluoro-4-nitro- phenol	2-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-6- fluoro-4-nitro-phenol	N-(4-{2-[(3-Fluoro-2-hydroxy-5- nitro-phenylamino)-methyl]- phenylsulfanyl}-phenyl)-acetamide	2-Fluoro-4-nitro-6-[2-(quinolin-7-ylsulfanyl)-benzylamino]-phenol
E S S	IN POON	E S S	NO <sub>2</sub> S NHAC	TZ O
472	473	474	475	476

477	P S S S S S S S S S S S S S S S S S S S	2-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-6-fluoro-4- nitro-phenol	C19H13CIFN3O5S	А	449.84	450.1
478	TZ SON	2-Fluoro-4-nitro-6-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	C20H16FN3O4S	Q	429.42	429.8
479	HZ SON	2-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-6- fluoro-4-nitro-phenol	C19H15CIFN3O2S	Д	419.86	420.2
480	TZ CO	2-[2-(4-Chloro-benzenesulfonyl)- benzylamino]-6-fluoro-4-nitro- phenol	C19H15CIFN2O5S	D	436.84	437.1

481	TZ TZ TZ	2,4-Dichloro-6-(3-phenoxy- benzylamino)-phenol	C19H15Cl2NO2	D	360.23	360.5
482	5 5 5	2,4-Dichloro-6-[3-(4-chloro- phenoxy)-benzylamino]-phenol	C19H15Cl3NO2	D	394.68	395.0
483	5 5	2-[3-(4-tert-Butyl-phenoxy)- benzylamino]-4,6-dichloro-phenol	C23H23Cl2NO2	D	416.34	416.8
484	12 5 5	2-(3-Benzyloxy-benzylamino)-4,6- dichloro-phenol	C20H17Cl2NO2	D	374.26	374.6

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485	12 5 5 5	2-(2-Benzyloxy-benzylamino)-4,6- dichloro-phenol	C20H17Cl2NO2	Д	374.26	374.6
486	\$	2,4-Dichlow-6-[(naphthalen-1- ylmethyl)-amino]-phenol	C17H13CI2NO	Q	318.20	318.6
487	TZ TO	2,4-Dichloro-6-(4-methylsulfanyl- benzylamino)-phenol	C14H13Cl2NOS	О	314.23	314.7
488	5—0 5—0	2,4-Dichloro-6-(2-ethylsulfanyl- benzylamino)-phenol	C15H15Cl2NOS	Q	328.26	328.6
489	-z	2,4-Dichloro-6-(2-morpholin-4-yl- benzylamino)-phenol	C17H18Cl2N2O2	Д	353.24	353.6

490	12 5 5	2,4-Dichloro-6-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	C17H12Cl3NOS2	D	416.77	416.9
491	Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z	2,4-Dichloro-6-[(5-phenyl-2H- imidazol-4-ylmethyl)-amino]- phenol	C16H13Cl2N3O	Q	334.20	334.6
492	TIN TO	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-4,6-dichloro- phenol	C11H8BrCl2NOS	Q	353.06	353.4
493	5 5	2,4-Dichloro-6-[3-(4-methoxy-phenoxy)-benzylamino]-phenol	C20H17Cl2NO3	D	390.26	390.6
494	5 0 0	2,4-Dichloro-6-(3-methyl- benzylamino)-phenol	C14H13Cl2NO	Q	282.17	282.4

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5	TX OF	2,4-Dichloro-6-(3-trifluoromethyl- benzylamino)-phenol	C14H10Cl2F3NO	D	336.14	336.5
5	55	2,4-Dichloro-6-(2-chloro-6-fluoro- benzylamino)-phenol	C13H9Cl3FNO	Ω	320.57	320.8
ğ—————————————————————————————————————		2,4-Dichloro-3-methyl-6-(3- phenoxy-benzylamino)-phenol	C20H17CIZNO2	Д	374.26	374.6
	5	2,4-Dichloro-3-methyl-6-[3-(4-chloro-phenoxy)-benzylamino]-phenol	C20H17Cl3NO2	Q	408.71	409.2

499	5 5 5	2-[3-(4-tert-Butyl-phenoxy)- benzylamino]-4,6-dichloro-3- methyl-phenoi	C24H25Cl2N02	D	430.37	430.5
200	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	2-(3-Benzyloxy-benzylamino)-4,6- dichloro-3-methyl-phenol	C21H19CI2NO2	Q	388.29	388.6
501	TZ TZ TZ	2-(2-Benzyloxy-benzylamino)-4,6- dichloro-3-methyl-phenol	C21H19ClZNO2	О	388.29	388.6
205	5 0 0	2,4-Dichloro-3-methyl-6- [(naphthalen-1-ylmethyl)-amino]- phenol	C18H15ClZNO	D	332.23	. 332.6

I	T			
328.6	342.8	367.6	431.2	348.8
328.26	342.29	367.27	430.80	348.23
О	D	Q	Q	D
CISHISCIZNOS	C16H17Cl2NOS	C18H20Cl2N2O2	C18H14Cl3NOS2	C17H15Cl2N3O
2,4-Dichloro-3-methyl-6-(4-methylsulfanyl-benzylamino)-phenol	2,4-Dichloro-3-methyl-6-(2- ethylsulfanyl-benzylamino)-phenol	2,4-Dichloro-3-methyl-6-(2- morpholin-4-yl-benzylamino)- phenol	2,4-Dichloro-3-methyl-6-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	2,4-Dichloro-3-methyl-6-[(5-phenyl-2H-imidazol-4-ylmethyl)-amino]-phenol
EN TO	ξσ	TZ 0	5 12 5 5	TZ TZ TZ TZ
503	504	505	909	507

₹———□	IZ STATE OF THE ST	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-4,6-dichloro-3- methyl-phenol	C12H10BrCl2NOS	Q	367.09	367.4
ğ		2,4-Dichloro-6-[3-(4-methoxy-phenoxy)-benzylamino]-3-methyl C21H19Cl2NO3 phenol	C21H19Cl2NO3	Ω	404.29	404.5
	12 5— 5	2,4-Dichloro-6-(3-methyl- benzylamino)-3-methyl-phenol	CISHISCIZNO	Д	296.20	296.8
5 5	IN TO THE PERSON OF THE PERSON	2,4-Dichloro-3-methyl-6-(3-trifluoromethyl-benzylamino)-phenol	C15H12Cl2F3NO	Ω	350.17	350.7
5	TZ TZ TZ	2,4-Dichloro-3-methyl-6-(2- chloro-6-fluoro-benzylamino)- phenol	C14H11Cl3FNO	Ð	334.60	335.0

326.1	. 360.6	382.2	340.1
325.79	360.23	381.90	339.82
D	Q	Q	Д
C19H16CINO2	C19H15CIZNO2	C23H24CINO2	C20H18CINO2
2-Chloro-6-(3-phenoxy-benzylamino)-phenol	2-Chloro-6-[3-(4-chloro-phenoxy)-benzylamino]-phenol	2-[3-(4-tert-Butyl-phenoxy)- benzylamino]-6-chloro-phenol	2-(3-Berzyloxy-benzylamino)-6- chloro-phenol
TZ B	5	5	5 J
513	514	515	516

<b>\</b>				
340.1	284.0	280.2	294.3	319.1
339.82	283.75	279.79	293.81	318.80
D	D	D	Q	. Д
C20H18CINO2	CI7H14CINO	C14H14CINOS	C15H16CINOS	C17H19CIN2O2
2-(2-Benzyloxy-benzylamino)-6- chloro-phenol	2-Chloro-6-[(naphthalen-1- ylmethyl)-amino]-phenol	2-Chloro-6-(4-methylsulfanyl- benzylamino)-phenol	2-Chloro-6-(2-ethylsulfanyl- benzylamino)-phenol	2-Chloro-6-(2-morpholin-4-yl- benzylamino)-phenol
E TEX	#Z #Z	E TZ	TN TO S	-z>
517	518	519	520	521

382.6	300.2	319.5	356.5	248.5
382.33	299.75	318.62	355.81	247.72
Q	Q	Д		Q
C17H13Cl2NOS2	C16H14CIN3O	C11H9BrCINOS	C20H18CINO3	C14H14CINO
2-Chloro-6-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	2-Chloro-6-[(5-phenyl-2H-imidazol-4-ylmethyl)-amino]-phenol	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-6-chloro-phenol	2-Chloro-6-[3-(4-methoxy-phenoy)-benzylamino]-phenol	2-Chloro-6-(3-methyl- benzylamino)-phenol
TN TO S	TZ TZ	H H H	1Z 5 0	TZ 5
522	523	524	525	526

302.2	286.6	309.8	344.0	366.0
301.69	286.13	309.33	343.77	365.44
D	Ω .	, Q	D	<b>Q</b> .
C14H11CIF3NO	C13H10Cl2FNO	C19H16FNO2	C19H15CIFNO2	C23H24FNO2
2-Chloro-6-(3-trifluoromethyl-benzylamino)-phenol	2-Chloro-6-(2-chloro-6-fluoro- benzylamino)-phenol	2-Fluoro-6-(3-phenoxy- benzylamino)-phenol	2-Fluoro-6-[3-(4-chloro-phenoxy)- benzylamino]-phenol	2-[3-(4-tert-Butyl-phenoxy)- benzylamino]-6-fluoro-phenol
E S	E TE	12 5	5	
527	528	529	530	531

				11 220
323.8	323.8	267.7	263.5	277.8
323.36	323.36	267.30	263.33	277.36
Q	D	D	Q	Q
C20H18FNO2	C20H18FNO2	C17H14FNO	C14H14FNOS	C15H16FNOS
2-(3-Benzyloxy-benzylamino)-6- fluoro-phenol	2-(2-Benzyloxy-benzylamino)-6- fluoro-phenol	2-Fluoro-6-[(naphthalen-1- ylmethyl)-amino]-phenol	2-Fluoro-6-(4-methylsulfanyl- benzylamino)-phenol	2-Fluoro-6-(2-ethylsulfanyl- benzylamino)-phenol
172 8-	5— ·	12/ 5-	E E	EZ E
532	533	534	535	536

302.8	366.0	283.8	302.5	339.8
302.34	365.87	283.30	302.16	339.36
D	Q	Q .	Q	Q
C17H19FN2O2	C17H13CIFNOS2	C16H14FN3O	C11H9BrFNOS	C20H18FNO3
2-Fluoro-6-(2-morpholin-4-yl- benzylamino)-phenol	2-Fluoro-6-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	2-Fluoro-6-[(5-phenyl-2H- imidazol-4-ylmethyl)-amino]- phenol	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-6-fluoro-phenol	2-Fluoro-6-[3-(4-methoxy-phenoxy)-benzylamino]-phenol
TZZ - 5	TIZ TO	Z Z TZ TO	IN HO	TZ TO
537	538	539	540	541

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542	E_F	2-Fluoro-6-(3-methyl-benzylamino)-phenol	C14H14FNO	Д	231.27	231.4
543	How have a second secon	2-Fluoro-6-(3-trifluoromethyl-benzylamino)-phenol	C14H11F4NO	Q	285.24	285.5
544	5 - 5	2-Fluoro-6-(2-chloro-6-fluoro- benzylamino)-phenol	C13H10CF2NO	D	269.67	270.1
545	5—————————————————————————————————————	2,3-Difluoro-6-(3-phenoxy- benzylamino)-phenol	C19H15F2NO2	D	327.32	327.6
546	5 -5	2,3-Difluoro-6-[3-(4-chloro- phenoxy)-benzylamino]-phenol	C19H14CIF2NO2	Ð	361.76	362.0

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383.8	341.7	341.7	285.6	281.6
383.43	341.35	341.35	285.29	281.32
Q	Д	О	Ð	Q
C23H23F2NO2	C20H17F2NO2	C20H17F2NO2	C17H13F2NO	C14H13F2NOS
2-[3-(4-tert-Butyl-phenoxy)- benzylamino]-5,6-difluoro-phenol	2-(3-Benzyloxy-benzylamino)-5,6- C20H17F2NO2 difluoro-phenol	2-(2-Benzyloxy-benzylamino)-5,6- difluoro-phenol	2,3-Difluoro-6-[(naphthalen-1-ylmethyl)-amino]-phenol	2,3-Difluoro-6-(4-methylsulfanyl- benzylamino)-phenol
TZ,	5—————————————————————————————————————	₹	TZ TO	TIN TO THE TIME TO
547	548	549	550	551

		2	9	4.
295.7	320.8	384.2	301.6	320.4
295.35	320.33	383.86	301.29	320.15
Q	O O	Ω	. Д	Q
CISHISFZNOS	C17H18F2N2O2	C17H12CIF2NOS2	C16H13F2N3O	C11H8BrF2NOS
2,3-Difluoro-6-(2-ethylsulfanyl- benzylamino)-phenol	2,3-Difluoro-6-(2-morpholin-4-yl- benzylamino)-phenol	2,3-Difluoro-6-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	2,3-Difluoro-6-[(5-phenyl-2H- imidazol-4-ylmethyl)-amino]- phenol	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-5,6-difluoro- phenol
TZ T	TZ T	E S S S S S S S S S S S S S S S S S S S	IZ H H	TZ T
552	553	554	555	556

357.6	249.6	303.7	288.1	347.0
357.35	249.26	303.23	287.66	346.23
О .	Q	Ω	Ð	Ø
	C14H13F2NO	C14H10F5NO	C13H9CIF3NO	C14H13Cl2NO3S
2,3-Difluoro-6-[3-(4-methoxy- phenoxy)-benzylamino]-phenol	2,3-Difluoro-6-(3-methyl- benzylamino)-phenol	2,3-Difluoro-6-(3-trifluoromethyl- benzylamino)-phenol	2,3-Difluoro-6-(2-chloro-6-fluoro- benzylamino)-phenol	N-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-C-phenyl- methanesulfonamide
5-\	TZ E	F TZ TS	\$	- NH O TO
557	558	559	999	561

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312.1	368.3	298.1	332.4	298.5
312.21	368.32	298.18	332.20	298.19
В	В	B	В	В
C11H15Cl2NO3S	CISHZ3Cl2NO3S	C10H13Cl2NO3S	C13H11Cl2NO3S	C10H13Cl2NO3S
Butane-1-sulfonic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide	Octane-1-sulfonic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide	Propane-2-sulfonic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide	N-(3,5-Dichloro-2-hydroxy- phenyl)-C-phenyl- methanesulfonamide	Butane-1-sulfonic acid (3,5-dichloro-2-hydroxy-phenyl)-amide
O S O TO	D IX OF	O S O O O	O O O O O O O O O O O O O O O O O O O	D NH O NH O
295	563	564	295	999

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354.6	284.5	297.9	264.0	320.3
354.29	284.16	297.76	263.74	319.85
В	В	Д	Ф	Ø
C14H21CIZNO3S	C9H11ClZNO3S	C13H12CINO3S	C10H14CINO3S	Ċ14HZ2CINO3S
Octane-1-sulfonic acid (3,5-dichloro-2-hydroxy-phenyl)-amide	Propane-2-sulfonic acid (3,5-dichloro-2-hydroxy-phenyl)-amide	N-(3-Chloro-2-hydroxy-phenyl)- C-phenyl-methanesulfonamide	Butane-1-sulfonic acid (3-chloro-2-hydroxy-phenyl)-amide	Octane-1-sulfonic acid (3-chloro- 2-hydroxy-phenyl)-amide
0 % 0 H	O HO TO	NHN DO	COHOSO	TZ O H
567	568	569	570	571

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	o to	Propane-2-sulfonic acid (3-chloro-2-hydroxy-phenyl)-amide	C9H12CINO3S	Ф	249.71	250.4
	TN-NHO HO	N-(3-Fluoro-2-hydroxy-phenyl)-C-phenyl-methanesulfonamide	C13H12FNO3S	Д	281.30	281.8
·	No. St. St. St. St. St. St. St. St. St. St	Butane-1-sulfonic acid (3-fluoro-2-hydroxy-phenyl)-amide	C10H14FNO3S	Д	247.29	247.8
	DO HOUSE	Octane-1-sulfonic acid (3-fluoro-2- hydroxy-phenyl)-amide	C14H22FNO3S	Д	303.39	303.8
1	O N HIN J	Propane-2-sulfonic acid (3-fluoro-2-hydroxy-phenyl)-amide	C9H12FNO3S	щ	233.26	233.7
1	N HN HO	N-(3,4-Difluoro-2-hydroxy- phenyl)-C-phenyl- methanesulfonamide	C13H11F2NO3S	В	299.29	300.8

		- 1		
265.7	321.8	251.6	320.2	306.4
265.28	321.38	251.25	320.22	306.18
В	В	В	F, G, H	F, G, H
C10H13FZNO3S	C14H21F2NO3S	C9H11F2NO3S	C14H19Cl2NO3	C13H17Cl2NO3
Butane-1-sulfonic acid (3,4-difluoro-2-hydroxy-phenyl)-amide	Octane-1-sulfonic acid (3,4-difluoro-2-hydroxy-phenyl)-amide	Propane-2-sulfonic acid (3,4-difluoro-2-hydroxy-phenyl)-amide	(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-carbamic acid hexyl ester	(3,5-Dichloro-2-hydroxy-phenyl)- carbamic acid hexyl ester
NHN HO	TZ OF	O S O HO	D P P	- OH
578	579	580	581	582

C13H18CINO3 F, G, H 271.74 272.1	NO3 F, G, H 255.29 255.6	334.5 F. G. H. 334.18 334.5	
	henyl)- C13H18FNO3	1ydroxy-   hexyl ester	
(3-Chloro-2-hydroxy-phenyl)-carbamic acid hexyl ester	(3-Fluoro-2-hydroxy-phenyl)-carbamic acid hexyl ester	(5-Bromo-3-fluoro-2-hydroxy- phenyl)-carbamic acid hexyl ester	
OF O	D. D. T. N.	HN OH OH	H.
583	584	585	

588	N N N N N N N N N N N N N N N N N N N	2-[3-(3,5-Dichloro-2-hydroxy-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	C15H20Cl2N2O4	¥	363.24	363.6
589	TIX O TIX TO TIX TO TIX	2-[3-(3-Chloro-2-hydroxy-phenyl)- ureido]-4-methyl-pentanoic acid ethyl ester	CISHZICINZO4	A	328.79	329.1
290	TZ O TZ O	2-[3-(3-Fluoro-2-hydroxy-phenyl)- ureido]-4-methyl-pentanoic acid ethyl ester	C15H21FN2O4	V	312.34	312.8
591	IZ O	2-[3-(3,4-Difluoro-2-hydroxy-4-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	C15H20F2N2O4	<b>∀</b>	330.33	330.8
592	H D D	2-[3-(5-Bromo-3-fluoro-2-hydroxy-4-methyl-phenyl)-ureido]-4-methyl-pentanoic acidethyl ester	C15H20BrFN2O4	4	391.23	391.6

593	IZ O	2-[3-(3,5-Dichloro-2-hydroxy-4- methyl-phenyl)-ureido]-3-phenyl- propionic acid ethyl ester	C19H20CI2N2O4	∢	411.28	411.1
594		2-[3-(3,5-Dichloro-2-hydroxy-phenyl-propionic acid ethyl ester	C18H18CIZN2O4	¥	397.25	397.6
595	TZ O	2-[3-(3-Chloro-2-hydroxy-phenyl)- ureido]-3-phenyl-propionic acid ethyl ester	acid C18H19CIN2O4	¥	362.81	363.0
969	TZ O	2-[3-(3-Fluoro-2-hydroxy-phenyi)- ureido]-3-phenyl-propionic acid ethyi ester	C18H19FN2O4	ď	346.35	346.7

364.8	425.6	332.5
364.34	425.25	332.27
Ą	₩	C, E
C18H18F2N2O4	C18H18BrFN2O4	C16H23CI2NO2
2-[3-(3,4-Difluoro-2-hydroxy-phenyl)-urcido]-3-phenyl-propionic acid ethyl ester	2-[3-(5-Bromo-3-fluoro-2-hydroxy-phenyl)-ureido]-3-phenyl-propionic acid ethyl ester	3,5,5-Trimethyl-hexanoic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide
TZ O	IZ O	5 5 5 7 5
597	598	599

Structure Chemical name Formula Synthesis MolWeight MS data  Compared to the c								
Comparison of the comparison o		Structure	Chemical name	Formula	Synthesis methods	MolWeight	MS data	
CONTRACTOR (3-5.5-Trimethyl-hexanoic acid (3-chloro-2-hydroxy-phenyl)-amide chloro-2-hydroxy-phenyl)-amide fluoro-2-hydroxy-phenyl)-amide closes (3-5.5-Trimethyl-hexanoic acid (3-chloro-2-hydroxy-phenyl)-amide closes (3-6-7.34 amide closes)  CONTRACTOR (3-6-7)-4-4-4-4-4-4-4-4-4-4-4-4-4-4-4-4-4-4-	009	\ \/	3,5,5-Trimethyl-hexanoic acid (3,5-dichloro-2-hydroxy-phenyl)- amide	C15H21Cl2NO2	C, B	318.24	318.5	
FOH H S.5.5-Trimethyl-hexanoic acid (3- G15H21FNO2 C, E 267.34 fluoro-2-hydroxy-phenyl)-amide C15H21F2NO2 C, E 267.34 amide C3.4-diffuoro-2-hydroxy-phenyl)- G15H21F2NO2 C, E 285.33	109	₹	3,5,5-Trimethyl-hexanoic acid (3-chloro-2-hydroxy-phenyl)-amide	C15H22CINO2	C, B	283.79	284.0	
F H C15HZ1FZNOZ C, E 285.33 amide	602		3,5,5-Trimethyl-hexanoic acid (3-fluoro-2-hydroxy-phenyl)-amide	C15H21FN02	C, B	267.34	267.7	
	603	₹	3,5,5-Trimethyl-hexanoic acid (3,4-difluoro-2-hydroxy-phenyl)-amide	CISHZIFZNOZ	ョ び	285.33	285.7	

346.5	383.4	439.8
346.24	382.88	438.99
д <b>,</b>	J followed by A	J followed by A
C15H21BrFNO2	C18H27CIN4O3	C22H35CIN4O3
3,5,5-Trimethyl-hexanoic acid (5-bromo-3-fluoro-2-hydroxy-phenyl)-amide	1-tert-Butyl-3-[3-chloro-5-(3- cyclohexyl-ureido)-2-hydroxy- phenyl]-urea	1-[3-Chloro-5-(3-cyclohexyl- ureido)-2-hydroxy-phenyl]-3- (1,1,3,3-tetramethyl-butyl)-urea
£	₹	NI N
28	905	909

517.4	450.9	426.4
516.48	449.97	426.31
J followed by D	J followed by D	J followed by D
C26H27Cl2N3O2S	C26H28CIN3O2	C20H22CI2FN3O2
1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-3-cyclohexylurea	1-{3-[(Biphenyl-2-ylmethyl)- amino]-5-chloro-4-hydroxy- phenyl}-3-cyclohexyl-urea	1-[3-Chloro-5-(2-chloro-6-fluoro-benzylamino)-4-hydroxy-phenyl]-3-cyclohexyl-urea
S S S S S S S S S S S S S S S S S S S	NT STORY	
607	809	609

404.9	406.8	406.8
404.89	405.88	405.88
J followed by A	J followed by G	J followed by G
C20H25CIN4O3	C20H24CIN3O4	C20H24CIN3O4
1-tert-Butyl-3-[3-chloro-2- hydroxy-5-(3-phenethyl-ureido)- phenyl]-urea	[3-Chloro-2-hydroxy-5-(3- phenethyl-ureido)-phenyl]- carbamic acid isobutyl ester	[3-Chloro-2-hydroxy-5-(3-phenethyl-ureido)-phenyll-carbamic acid sec-butyl ester
TZ NH	PO ONH	HO NH
. 610	611	612

401.9	415.9	413.8
401.89	415.92	412.95
J followed by C	J followed by C	J followed by A
C21H24CIN3O3	C22H26CIN3O3	C20H33CIN4O3
Cyclopentanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenethylureido)-phenyl]-amide	Cyclohexanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenethylureido)-phenyl]-amide	1-tert-Butyl-3-{3-chloro-2- hydroxy-5-[3-(1,1,3,3-tetramethyl- butyl)-ureido]-phenyl}-urea
TIN O NH	TIN ON NH	D IN O NI
613	614	615

	T	
413.8	414.1	381.9
413.94	413.94	381.90
J followed by G	J followed by G	J followed by C
C20H32CIN3O4	C20H32CIN3O4	C19H28CIN3O3
{3-Chloro-2-hydroxy-5-[3- (1,1,3,3-tetramethyl-butyl)- ureido]-phenyl}-carbamic acid isobutyl ester	(3Chloro-2-hydroxy-5-[3- (1,1,3,3-tetramethyl-butyl)- ureido]-phenyl}-carbamic acid sec- butyl ester	Cyclopropanecarboxylic acid {3-chloro-2-hydroxy-5-[3-(1,1,3,3-tetramethyl-butyl)-ureido]-phenyl}-amide
D NH NH	PO NH	D IZ O NH
. 616	617	618

410.1	424.0
409.95	423.98
J followed by C	J followed by
C21H32CIN3O3	C22H34CIN3O3
Cyclopentanecarboxylic acid {3-chloro-2-hydroxy-5-[3-(1,1,3,3-tetramethyl-butyl)-ureido]-phenyl}-amide	Cyclohexanecarboxylic acid {3-chloro-2-hydroxy-5-[3-(1,1,3,3-tetramethyl-butyl)-ureido]-phenyl}-amide
D NH NH	HO NH
620	621
	Cyclopentanecarboxylic acid {3-chloro-2-hydroxy-5-[3-(1,1,3,3-teramethyl-butyl)-ureido]-tetramethyl-amide

389.9	390.8	390.8
389.88	390.86	390.86
L followed by A	L followed by G	L followed by G
C20H24CIN3O3	C20H23CIN2O4	C20H23CIN2O4
N-[3-(3-tert-Butyl-ureido)-5- chloro-4-hydroxy-phenyl]-3- phenyl-propionamide	[3-Chloro-2-hydroxy-5-(3-phenyl-propionylamino)-phenyl]-carbamic acid isobutyl ester	[3-Chloro-2-hydroxy-5-(3-phenyl- propionylamino)-phenyl]-carbamic acid sec-butyl ester
TZ O B		HO HO NH
	623	624

-		
358.9	373.8	386.8
358.82	372.85	386.87
L followed by C	L followed by	L followed by
C19H19CIN2O3	C20H21CIN2O3	C21H23CIN2O3
Cyclopropanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenyl-propionylamino)-phenyl]-amide	Cyclobutanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenyl-propionylamino)-phenyl-amide	Cyclopentanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenyl-propionylamino)-phenyl]-amide
TZ 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	E N	E S
. 529	979	627

401.8	319.7	342.3
400.90	319.25	341.85
L followed by C	I	Q
C22H24CIN2O3	C13H16Cl2N2OS	C19H16CINOS
Cyclohexanecarboxylic acid [3-chloro-2-hydroxy-5-(3-phenylpropionylamino)-phenyl]-amide	1-Cyclopentyl-3-(3,5-dichloro-2-hydroxy-4-methyl-phenyl)-thiourea	2-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-phenol
5 E	TZ S	S IN S
	629	630

525.1	539.1	545.5
524.46	538.49	544.88
J followed by D	J followed by D	J followed by D
CZ7HZ3Cl2N3O2S	C28H25CI2N3O2S	C26H20Cl3N3O2S
1-Benzyl-3-[3-chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-urea	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-3-phenethyl-urea	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-3-(4-chloro-phenyl)-urea
\$\frac{1}{2} \frac{5}{2} \frac{5}{2} \frac{5}{2} \frac{1}{2} \frac	N SI	NH NH NH
631	e32 c	633

376.1	382.2	376.1
375.9	381.90	375.9
J followed by B	J followed by	K followed by A
C15H22CIN3O4S	C19H28CIN3O3	C18H18CIN3O2S
Ethanesulfonic acid [3-chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-amide	N-[3-Chloro-5-(3-cyclohexyl- ureido)-2-hydroxy-phenyl]-3,3- dimethyl-butyramide	1-(5-Benzothiazol-2-yl-3-chloro-2- hydroxy-phenyl)-3-tert-butyl-urea
NH ON NH		TZ Z
634	635	636

_	101	
410.1	424.1	378.1
409.9	423.9	377.9
K followed by A	K followed by A	K followed by
C21H16CIN3O2S	C22H18CIN3O2S	C17H16CIN3OS2
1-(5-Benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-3-benzyl-urea	1-(5-Benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-3-phenethyl-urea	1-(5-Benzothiazol-2-yl-3-chloro-2- hydroxy-phenyl)-3-isopropyl- thiourea
EZ O Z		TIZ NO TIZ
637	638	639

392.1	417.2	409.2	256.9
391.9	417.0	408.9	263.31
K followed by I	K followed by C	K followed by C	<b>V</b>
C18H18CIN3OS2	C22H25CIN2O2S	C22H17CIN2O2S	C13H20N2O2
1-(5-Benzothiazol-2-yl-3-chloro-2- hydroxy-phenyl)-3-tert-butyl- thiourea	3,5,5-Trimethyl-hexanoic acid (5-benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-amide	N-(5-Benzothiazol-2-yl-3-chloro- 2-hydroxy-phenyl)-3-phenyl- propionamide	1-(2-Hydroxy-4-methyl-phenyl)-3- pentyl-urea
IZ Z Z	NH NO	N HO	P IN
640	128	642	643

350.5	336.5	303.6	580.9
350.16	336.14	303.23	580.31
D	Q	D	J followed by D
CISH12CIZF3NO	C14H10C12F3NO	C14H10F5NO	C25H18Cl4N4O2S
2,4-Dichloro-3-methyl-6-(2-trifluoromethyl-benzylamino)-phenol	2,4-Dichloro-6-(2-trifluoromethyl-benzylamino)-phenol	2,3-Difluoro-6-(2-trifluoromethyl-benzylamino)-phenol	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-3-(2,6-dichloro-pyridin-4-yl)-urea
5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	# # # # # # # # # # # # # # # # # # #	5-Z-5-5-5-5-5-5-5-5-5-5-5-5-5-5-5-5-5-5
649	059	651	652

404.6	520.1	282.7	379.9
403.95	519.44	282.17	379.24
K followed by	J followed by D	D	¥
C19H18CIN3OS2	C24H24Cl2N4O3S	C14H13Cl2NO	C17H16Cl2N4O2
1-(5-Benzothiazol-2-yl-3-chloro-2- hydroxy-phenyl)-3-cyclopentyl- thiourea	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-4-hydroxy-phenyl}-3-morpholin-4-yl-urea	6-Benzylamino-2,4-dichloro-3- methyl-phenol	1-[2-(1H-Benzoimidazol-2-yl)- ethyl]-3-(3,5-dichloro-2-bydroxy- 4-methyl-phenyl)-urea
E S S S S S S S S S S S S S S S S S S S	S S S S S S S S S S S S S S S S S S S	2 2 2 2 3	IZ O IZ O
653	654	655	929

404.6	384.4	398.2	418.9
403.95	383.89	397.92	418.34
K followed by I	Q	Q	. Ω
C19H18CIN3OS2	C21H18CINO2S	C22HZ0CINO2S	C21H17CI2NO2S
1-(5-Benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-3-cyclopentyl-thiourea	1-[5-Chloro-2-hydroxy-3-(2-phenylsulfanyl-benzylamino)-phenyl]-ethanone	1-[5-Chloro-2-hydroxy-3-(2-p-tolylsulfanyl-benzylamino)-phenyl]-ethanone	1-{5-Chloro-3-[2-(4-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone
E S S S S S S S S S S S S S S S S S S S	0 — 0 — 0 — 0 — 0 — 0 — 0 — 0 — 0 — 0 —	TZ TO O	TZ 5
657	859	629	099

429.3	414.3	418.9	418.8	453.2
428.89	413.92	418.34	418.34	452.78
D	Q	D	Ω.	Д
C21H17CIN2O4S	C22H20CINO3S	C21H17Cl2NO2S	C21H17Cl2NO2S	C21H16Cl3NO2S
1-{5-Chioro-2-hydroxy-3-[2-(4- nitro-phenylsulfanyl)- benzylamino]-phenyl}-ethanone	1-{5-Chloro-2-hydroxy-3-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenyl}-ethanone	1-{5-Chloro-3-[2-(2-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	1-{5-Chloro-3-[2-(3-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	1-{5-Chloro-3-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone
5 5 5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	TZ TO	5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	5 -5 -5 -0	5 5 5 0 12 0
199	799	663	664	999

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o=<	5 5 5	N-(4-{2-[(3-Acetyl-5-chloro-2-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide	C23H21CIN2O3S	Q	440.94	441.4
	2 3 5 5 0	1-{5-Chloro-2-hydroxy-3-[2- (quinolin-7-ylsulfanyl)- benzylamino]-phenyl}-ethanone	C24H19CIN2O2S	Ω .	434.94	435.3
`	5 0 0 0	1-{5-Chloro-3-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-2-hydroxy-phenyl}-ethanone	C21H16Cl2N2O4S	Q	463.33	463.9
		1-[5-Chloro-2-hydroxy-3-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenyl]-ethanone	C22H19CIN2O4S	Q	442.92	443.3

1-{3-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-5-chloro-2-hydroxy-phenyl}-c21H18Cl2N2O2S D ethanone
1-{5-Chloro-3-[2-(4-chloro-benzylamino]-2-hydroxy-phenyl}-ethanone
4-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-benzene-1,3-diol
1,6-Di-(3,5-Dichloro-2-hydroxy-4- C22H26Cl4N4O4 A followed by methyl-phenyl)-3-hexyl-urea
3-[3-(3-Chloro-4-hydroxy-phenyl)- ureido]-propionic acid ethyl ester

256.9	276.9	290.9	291.2	299.4	243.0
256.73	276.72	290.74	290.75	298.81	242.70
A	Ą	¥	Ą	Ä	∢
C12H17CIN2O2	C14H13CIN2O2	C15H15CIN2O2	C15H15CIN2O2	C15H23CINZO2	C11H15CIN2O2
1-(3-Chloro-4-hydroxy-phenyl)-3- pentyl-urea	1-Benzyl-3-(3-chloro-4-hydroxy-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (2-methyl-benzyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- phenethyl-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-(3-chloro-4- hydroxy-phenyl)-urea
IX OF	TZ OF	IZ OF	IZ OF	IZ OF	TX OH
675	929	119	879	629	089

170

283.1	345.0	331.9	297.7	331.0	269.1
282.77	344.72	331.59	297.14	330.69	268.74
¥	ď	¥	Ą	. <b>4</b>	4
C14H19CIN2O2	C15H12CIF3N2O2	C13H9Cl3NZO2	C13H10CI2N2O2	C14H10CIF3N2O2	C13H17CIN2O2
1-(3-Chloro-4-hydroxy-phenyl)-3- cyclohexylmethyl-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	1-(3-Chloro-3-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-chloro-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- cyclohexyl-urea
IZ OF	IN OF OTHER PROPERTY OF THE PR	D IX OH	TZ OH	TX O TX	IZ O TO
681	682	683	684	589	989

<b>&gt;=</b> 0	ocfs	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-trifluoromethoxy-phenyl)-urea	C14H10CIF3N2O3	Ą	346.69	346.9
IZ O	\$	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-cyano-phenyl)-urea	C14H10CIN3O2	. ◆	287.70	287.9
IZ OF		1-Benzo[1,3]dioxol-5-yl-3-(3- chloro-4-hydroxy-phenyl)-urea	C14H11CINZO4	<b>∀</b>	306.70	306.9
HZ O		1-(3-Chloro-4-hydroxy-phenyl)-3- o-tolyl-urea	C14H13CIN2O2	ď	276.72	276.9
TZ OF	OMB	1-(3-Chioro-4-hydroxy-phenyl)-3- (3-methoxy-phenyl)-urea	C14H13CIN2O3	∢ .	292.72	292.9
IZ O		1-(3-Chloro-4-hydroxy-phenyl)-3- (2,6-dimethyl-phenyl)-urea	C15H15CIN2O2	<b>∀</b>	290.75	290.9
5						

353.2	313.1	321.4	354.9	263.2
352.77	312.75	320.82	354.79	262.70
А	4	¥	A	. ч
C16H17CIN2O5	C17H13CIN2O2	C17H21CIN2O2	C19H15CINZO3	C13H11CIN2O2
1-(3-Chloro-4-hydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- naphthalen-1-yl-urea	i-Adamantan-1-yl-3-(3-chloro-4-hydroxy-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-phenoxy-phenyl)-urea	1-(3-Chloro-4-hydroxy-phenyl)-3- phenyl-urea
HO Ne OMe	-D IZ O	-5 -5 P	TZ O	IN O TO
693	. 694	969	969	269

869	O HO DH	3-[3-(3,5-Dichloro-4-hydroxy-phenyl)-ureido]-propionic acid ethyl ester	acid C12H14Cl2N2O4	A	321.16	321.9
669	IN OH	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-pentyl-urea	C12H16CI2N2O2	∢	291.17	292.0
700	D IN D	1-Benzyl-3-(3,5-dichloro-4- hydroxy-phenyl)-urea	C14H12Cl2N2O2	<b>∀</b>	311.16	312.0
701	TZ O	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea	C15H14Cl2N2O2	ď	325.19	325.9
702	IZ O TZ O TZ	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-phenethyl-urea	C15H14Cl2N2O2	. <b>A</b>	325.19	325.9
703	IZ O TZ O TZ	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-urea	C15H22CI2N202	A	333.25	334.0

<b>∞</b>		∞	o;	6.	6.3
277.8	318.1	379.8	366.9	331.9	365.9
277.15	317.21	379.16	366.03	331.58	365.13
∢	¥	¥	Ą	. <b>4</b>	∢
C11H14Cl2N2O2	C14H18Cl2N2O2	C15H11CI2F3N2O2	C13H8Cl4N2O2	C13H9Cl3N2O2	C14H9ClZF3N2O2
1-tert-Butyl-3-(3,5-dichloro-4- hydroxy-phenyl)-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-cyclohexylmethyl-wea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(4-chloro-phenyl)-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea
JZ O T	IN OH	D H D D D D D D D D D D D D D D D D D D	TZ O	TIN OF TO	TZ OF
<b>2</b> 6	705	706	707	708	709

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304.0	381.8	322.9	341.7	311.8	327.5
303.18	381.13	322.15	341.15	311.16	327.16
¥	∢	Ą	∢	Α .	¥
C13H16Cl2N2O2	C14H9Cl2F3N2O3	C14H9ClZN3O2	C14H10Cl2N2O4	C14H12Cl2N2O2	C14H12Cl2N2O3
1-(3,5-Dichloro-4-hydroxy- phenyl)-3-cyclohexyl-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-trifluoromethoxy- phenyl)-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3,5-dichloro-4-hydroxy-phenyl)-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-o-tolyl-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(3-methoxy-phenyl)- urea
TN OF	TN. OOF3	D IN O	IZ O OH		D H O H
710	711	712	713	714	715

325.6	387.6	347.6	355.7	389.6
325.19	387.21	347.20	355.26	389.23
A	A	¥	<b>V</b>	A
C15H14Cl2N2O2	C16H17CI2N2O5	C17H12CI2N2O2	C17HZ0Cl2N2O2	C19H14Cl2N2O3
1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(2,6-dimethyl-phenyl)-	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(3,4,5-trimethoxy-phenyl)-urea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(3,5-dichloro-4-hydroxy-phenyl)-urea	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(4-phenoxy-phenyl)-urea
D TZ OT	HO NOMe	IZ DEO	D HV O	CI N N N N N N N N N N N N N N N N N N N
716	717	718	719	720

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297.7	297.8	267.9	287.9	301.8	301.8	309.8
297.14	297.26	267.28	287.27	301.30	301.30	309.36
A	A	Ą	¥	A	. <b>V</b>	Ą
C13H10Cl2N2O2	C12H15N3O6	C12H17N3O4	C14H13N3O4	C15H15N3O4	C15H15N3O4	C15H23N3O4
1-(3,5-Dichloro-4-hydroxy- phenyl)-3-phenyl-urea	3-[3-(4-Hydroxy-3-nitro-phenyl)- ureido]-propionic acid ethyl ester	1-(4-Hydroxy-3-nitro-phenyl)-3- pentyl-urea	1-Benzyl-3-(4-hydroxy-3-nitro- phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (2-methyl-benzyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- phenethyl-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea
HA CO	IN OH	N.O. HA OH	IN NO	IN OO	IN O	HZ OH
721	722	723	724	725	726	727

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253.8	293.9	355.8	342.7	308.4	341.8	279.8
253.25	293.32	355.27	342.13	307.69	341.24	279.29
A	Ą	∢	<b>V</b>	A	. <b>4</b>	4
C11H15N3O4	C14H19N3O4	CISH12F3N3O4	C13H9C12N3O4	C13H10CIN3O4	C14H10F3N3O4	C13H17N3O4
1-tert-Butyl-3-(4-hydroxy-3-nitro- phenyl)-urea	1-Cyclohexylmethyl-3-(4- hydroxy-3-nitro-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	1-(3,5-Dichloro-phenyl)-3-(4- hydroxy-3-nitro-phenyl)-urea	1-(4-Chloro-phenyl)-3-(4-hydroxy-3-nitro-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (4-trifluoromethyl-phenyl)-urea	1-Cyclohexyl-3-(4-hydroxy-3- nitro-phenyl)-urea
IN O I	N O H	O <sub>2</sub> N H N O <sub>2</sub> N H	D OH	IN O	O <sub>2</sub> N N N O N O OF S	O <sub>P</sub> N H O <sub>P</sub> O <sub>P</sub> N
728	729	730	731	732	733	734

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357.9	298.9	317.9	287.9	303.8	301.9	364.0
357.24	298.25	317.25	287.27	303.27	301.30	363.32
¥	Ą	¥	ď	<b>∀</b>	₹ .	A
C14H10F3N3O5	C14H10N4O4	C14H11N3O6	C14H13N3O4	C14H13N3O5	C15H15N3O4	C16H17N3O7
1-(4-Hydroxy-3-nitro-phenyl)-3- (4-trifluoromethoxy-phenyl)-urea	1-(4-Cyano-phenyl)-3-(4-hydroxy- 3-nitro-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(4- hydroxy-3-nitro-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3-o- tolyl-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (3-methoxy-phenyl)-urea	1-(2,6-Dimethyl-phenyl)-3-(4- hydroxy-3-nitro-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea
O <sub>2</sub> N H H OOF <sub>3</sub>	N <sub>e</sub> O H	O N N N N O H	HZ O HZ	O <sub>2</sub> N N N O <sub>M</sub> e	HN O OH	O <sub>2</sub> N H N OMe
735	736	737	738	739	740	741

323.9	331.9	366.0	273.9	270.6	240.5	260.8
323.30	331.37	365.34	273.24	270.26	240.27	260.26
∢	Ą	Ą	¥	¥	. ∢	¥
C17H13N3O4	C17H21N3O4	C19H15N3O5	C13H11N3O4	C12H15FN2O4	C12H17FN2O2	C14H13FN2O2
1-(4-Hydroxy-3-nitro-phenyl)-3- naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(4-hydroxy- 3-nitro-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- (4-phenoxy-phenyl)-urea	1-(4-Hydroxy-3-nitro-phenyl)-3- phenyl-urea	3-[3-(3-Fluoro-4-hydroxy-phenyl)- ureido]-propionic acid ethyl ester	1-(3-Fluoro-4-hydroxy-phenyl)-3- pentyl-urea	1-Benzyl-3-(3-fluoro-4-hydroxy- phenyl)-urea
N <sub>2</sub> O <sub>2</sub> N <sub>N</sub> O <sub>H</sub>	HZ OH	IZ	N O N O O O O O O O O O O O O O O O O O	HZ OH	IN OH	IN SECOND
742	743	744	745	746	747	748

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274.9	274.6	282.9	226.5	266.7	328.4	315.5
274.29	274.29	282.35	226.25	266.31	328.26	315.13
A	A	А	¥	¥	Ą	¥
C15H15FN2O2	C15H15FN2O2	C15H23FN2O2	C11H15FN2O2	C14H19FN2O2	C15H12F4N2O2	C13H9Cl2FN2O2
1-(3-Fluoro-4-hydroxy-phenyl)-3- (2-methyl-benzyl)-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- phenethyl-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-(3-fluoro-4- hydroxy-phenyl)-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- cyclohexylmethyl-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-urea
IZ O		TZ O			IN I	DI NOTE OF THE PERSON OF THE P
749	750	751	752	753	754	755

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781 1	7.107	314.6	252.6	330.5	271.5	290.7	260.5	276.5
67 000	780.00	314.24	252.28	330.23	271.25	290.25	260.26	276.26
	<b>4</b>	A	Ą	₩	4	¥	A	A
	C13H10CIFN202	C14H10F4N2O2	C13H17FN2O2	C14H10FF3N2O3	C14H10FN3O2	C14H11FN2O4	C14H13FN2O2	C14H13FN2O3
1 (2 Ellenny / herdenver-mhenvill-3-	1-(3-Finony-raymony)-promy (4-chloro-phenyl)-urea	1-(3-Fluoro-2-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- cyclohexyl-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-trifluoromethoxy-phenyl)-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3- fluoro-4-hydroxy-phenyl)-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- o-tolyl-urea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (3-methoxy-phenyl)-urea
. ZZ	5	HO N OF S	IZ O	HOOF <sub>2</sub>	IZ O	IZ ST	IZ O	HO NH OMB
	756	757	758	759	760	761	762	763

764		1-(3-Fluoro-4-hydroxy-phenyl)-3- (2,6-dimethyl-phenyl)-urea	C15H15FN2O2	∢	274.29	274.7
765	F OMe OMe	1-(3-Fluoro-4-hydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea	C16H17FN2O5	Ą	336.31	336.6
992	IN OH	1-(3-Fluoro-4-hydroxy-phenyl)-3- naphthalen-1-yl-urea	C17H13FNZO2	4	296.3	296.6
191	IZ O	1-Adamantan-1-yl-3-(3-fluoro-4- hydroxy-phenyl)-urea	C17H21FN2O2	<b>4</b>	304.36	304.6
892	IN N N	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-phenoxy-phenyl)-urea	C19H15FN2O3	<b>V</b>	338.33	338.6
692	IZ O	1-(3-Fluoro-4-hydroxy-phenyl)-3- phenyl-urea	C13H11FN2O2	¥	246.24	246.5

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268.7	238.6	258.6	272.5	272.5	280.7	224.8
268.27	238.28	258.27	272.30	272.30	280.36	224.26
Ą	∢	∢ .	<b>4</b>	¥	. <b>V</b>	4
C12H16N2O5	C12H18N2O3	C14H14N2O3	C15H16N2O3	C15H16N2O3	C15H24N2O3	C11H16N2O3
3-[3-(2,4-Dihydroxy-phenyl)- ureido]-propionic acid ethyl ester	1-(2,4-Dihydroxy-phenyl)-3- pentyl-urea	1-Benzyl-3-(2,4-dihydroxy- phenyl)-urea	1-(2,4-Dihydroxy-phenyl)-3-(2- methyl-benzyl)-urea	1-(2,4-Dihydroxy-phenyl)-3- phenethyl-urea	1-(2,4-Dihydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-(2,4-dihydroxy- phenyl)-urea
JIN OF OF	HA OF	IZ F	IZ O	HO HO HO	IN O	HN OH
170	771	772	773	774	775	9/1

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<b></b>	HO IN OF	1-Cyclohexylmethyl-3-(2,4-dihydroxy-phenyl)-urea	C14H20N2O3	Ą	264.32	264.7
	HO H	1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethyl-benzyl)-urea	CI5H13F3N2O3	¥	326.27	326.8
	PZ OF	1-(3,5-Djchloro-phenyl)-3-(2,4- dihydroxy-phenyl)-urea	C13H10Cl2N2O3	∢	313.14	313.7
	HO OH	1-(4-Chloro-phenyl)-3-(2,4- dihydroxy-phenyl)-urea	C13H11CIN2O3	¥	278.69	279.2
<del> </del>	IN OH	1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethyl-phenyl)-urea	C14H11F3N2O3	<b>V</b>	312.24	312.8
	EZ O	1-Cyclohexyl-3-(2,4-dihydroxy-phenyl)-urea	C13H18N2O3	A	250.29	250.8
	2					

	IN OOH	1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethoxy-phenyl)-urea	C14H11F3N2O4	₹	328.24	328.7
	#Z # # # # # # # # # # # # # # # # # #	1-(4-Cyano-phenyl)-3-(2,4- dihydroxy-phenyl)-urea	C14H11N3O3	Ą	269.26	269.8
	HV HO OH	1-Benzo[1,3]dioxol-5-yl-3-(2,4- dihydroxy-phenyl)-urea	C14H12N2O5	4	288.26	288.9
	IZ IZ IZ	1-(2,4-Dihydroxy-phenyl)-3-o- tolyl-urea	C14H14N2O3	ď	258.27	258.7
	HO HO OH	1-(2,4-Dihydroxy-phenyl)-3-(3- methoxy-phenyl)-urea	C14H14N2O4	A	274.27	274.8
	IZ D TZ D TZ	1-(2,4-Dihydroxy-phenyl)-3-(2,6- dimethyl-phenyl)-urea	C15H16N2O3	. <b>4</b>	272.30	272.9
<u> </u>	HO HO OM8	1-(2,4-Dihydroxy-phenyl)-3- (3,4,5-trimethoxy-phenyl)-urea	C16H18N2O6	¥	334.32	334.8

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400.4	414.5	414.4	422.5	366.4	406.5
400.07	414.09	414.09	422.16	366.05	406.11
¥	<b>∀</b>	¥	¥	· A	¥
C14H12B/2N2O2	C15H14Br2N2O2	C15H14Br2N2O2	C15H22Br2N2O2	C11H14Br2N2O2	C14H18Br2N2O2
1-Benzyl-3-(3,5-Dibromo-4- hydroxy-phenyl)-urea	1-(5-Bromo-3-fluoro-2-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-phenethyl-urea	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-(3,5-dibromo-4- hydroxy-phenyl)-urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-cyclohexylmethyl-urea
IN OH	HN OH	IN OH	IN OH	IX Of IX	IN O
796	797	798	799	800	801

802 Bright Holy Cors phenyl)-3-(4-miltoromethyl- C15H11Br2F3NZO2 A 468.06 phenyl)-3-(4-miltoromethyl- C13HBBr2CIZNZO2 A 454.93 phenyl)-3-(3,5-dichloro-phenyl)- C13HBBr2CIZNZO2 A 454.93 phenyl)-3-(3,5-dichloro-phenyl)- C13HBBr2CIZNZO2 A 454.04 phenyl)-3-(4-chloro-phenyl)-urea Bright Holy phenyl)-3-(4-chloro-phenyl)-urea phenyl)-3-(4-chloro-phenyl)-urea phenyl)-3-(4-chloro-phenyl)-urea phenyl)-3-(4-chloromethyl- C13HBBr2CIZNZO2 A 454.04 phenyl)-3-(4-chloromethyl- C13HBBr2NZO2 A 392.09 phenyl)-3-(4-miltoromethoxy- C14HBBr2NZO2 A 454.04 phenyl)-3-(4-miltoromethoxy- C14HBBr2NZO2 A 470.04 phenyl)-3-(4-miltoromethoxy- C14HBBr2NZO3 A 470.04 phenyl)-3-(4-miltoromethoxy-							
BY THE BEACTING A BANDIN-3-(3,5-dichloro-phenyl)-  BY THE BEACTING A BANDIN-3-(3,5-dichloro-phenyl)-  BY THE BY TH	8 .	IZ T	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	C15H11Br2F3N2O2	Ą	468.06	468.4
BIT HOLD THE BOOKES  BY HOLD THE BOOKES  BIT HOLD T	603	IZ a	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea	C13H8Br2Cl2N2O2	∢	454.93	455.4
Bry How How How Holls and Artifluoromethyles and How How Holls and How Holls and Holls	2	IZ DO IZ	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-chloro-phenyl)-urea	C13H9BrZCIN2O2	∢	420.48	420.7
Br HO HO CI3HIGBr2N202 A Dibromo-4-hydroxy- C13HIGBr2N202 A Dibromo-4-hydroxy- C13HIGBr2N202 A I-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-trifluoromethoxy- phenyl)-3-(4-trifluoromethoxy- phenyl)-area Professional Prof	805	IZ.	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea	C14H9Br2F3N2O2	¥	454.04	454.3
Br HO HO CoF <sub>3</sub> phenyl)-3-(4-trifluoromethoxy- C14H9Br2F3N2O3 A phenyl)-urea	908		1-(3,5-Dibromo-4-hydroxy- phenyl)-3-cyclohexyl-urea	C13H16Br2N2O2	A	392.09	392.5
	807	IZ bis	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(4-trifluoromethoxy-phenyl)-urea	C14H9Br2F3N2O3	A	470.04	470.3

808	HA OH	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	C14H9Br2N3O2	Ą	411.05	411.5
808	TN OH	1-Benzo[1,3]dioxol-5-yl-3-(3,5- dibromo-4-hydroxy-phenyl)-urea	C14H10Br2N2O4	¥	430.05	430.3
810	IN DH	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-o-tolyl-urea	C14H12Br2N2O2	<b>∀</b>	400.07	400.4
811	HO H	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(3-methoxy-phenyl)-	C14H12Br2N2O3	∢	416.06	416.3
812		1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(2,6-dimethyl-phenyl)-	C15H14Br2N2O2	Α.	414.09	414.5
813	Br N HO OMB	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(3,4,5-trimethoxy-phenyl)-urea	C16H17Br2N2O5	A	476.12	476.4

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436.4	444.2	478.3	386.2	288.9
436.10	444.16	478.13	386.04	288.25
<b>∀</b>	¥	A	¥	. <b>V</b>
C17H12Br2N2O2	C17H20Br2N2O2	C19H14Br2N2O3	C13H10Br2N2O2	C12H14F2N2O4
1-(3,5-Dibromo-4-hydroxy- phenyl)-3-naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(3,5-dibromo- 4-hydroxy-phenyl)-urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-phenoxy-phenyl)- urea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-phenyl-urea	3-[3-(3,5-Difluoro-4-hydroxy-phenyl)-ureido]-propionic acid ethyl ester
HV OH	HN OH	HO HO NEW TO THE TOTAL THE TOTAL TO THE TOTAL TOTAL TO THE TOTAL TO THE TOTAL TO THE TOTAL TO THE TOTAL TO TH	TZ O TZ	
814	815	816	817	818

258.9	278.8	292.9	292.9	300.5	244.3
258.26	278.25	292.28	292.28	300.34	244.24
₹	∢	Ą	¥	· <b>V</b>	<b>V</b>
C12H16F2N2O2	C14H12F2N2O2	C15H14F2N2O2	C15H14F2N2O2	C15H22F2N2O2	C11H14F2N2O2
1-(3,5-Difluoro-4-hydroxy- phenyl)-3-pentyl-urea	1-Benzyl-3-(3,5-difluoro-4- hydroxy-phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(2-methyl-benzyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-phenethyl-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(1,1,3,3-tetramethyl- butyl)-urea	1-tert-Butyl-3-(3,5-difluoro-4- hydroxy-phenyl)-urea
IZ OF	IZ O	IZ U U U U U U U	IZ D IZ D IZ	IN OH	IX OH
819	820	821	822	823	824

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284.6	346.5	333.3	298.9	332.7	270.7
284.30	346.25	333.12	298.67	332.23	270.28
Ą	Ą	Ą	∢	· <b>V</b>	A
C14H18F2N2O2	C15H11F5N2O2	C13H8Cl2F2N2O2	C13H9CIF2N2O2	C14H9F5N2O2	C13H16F2N2O2
1-(3,5-Difluoro-4-hydroxy- phenyl)-3-cyclohexylmethyl-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-chloro-phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-cyclohexyl-urea
IZ P	TN OF THE PERSON	TZ O TZ	TZ O TZ	HO LOFE S	TX OH
825	826	827	828	829	830

				<del></del>	<del></del>
348.6	289.5	308.5	278.6	294.5	292.6
348.22	289.24	308.24	278.25	294.25	292.28
А	Ą	¥	∢	Α.	A
C14H9F2F3N2O3	C14H9F2N3O2	C14H10F2N2O4	C14H12F2N2O2	C14H12F2N2O3	C15H14F2N2O2
1-(3,5-Difluoro-4-hydroxy-phenyl)-3-(4-trifluoromethoxy-phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-cyano-phenyl)-urea	1-Benzo[1,3]dioxol-5-yl-3-(3,5-difluoro-4-hydroxy-phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-o-tolyl-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(3-methoxy-phenyl)- urea	1-(3,5-Difluoro-4-hydroxy- · phenyl)-3-(2,6-dimethyl-phenyl)- urea
HO NH	IZ O IZ U U	TN OH	IZ O IZ	HO NHOWE	IZ OH
831	832	833	834	835	836

354.6	314.6	322.7	356.6	264.7
354.31	314.29	322.35	356.32	264.23
٧	Ą	<b>∀</b>	Ą	. <b>V</b>
C16H17F2N2O5	C17H12F2N2O2	C17H20F2N2O2	C19H14F2N2O3	C13H10F2N2O2
1-(3,5-Difluoro-4-hydroxy-phenyl)-3-(3,4,5-trimethoxy-phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-naphthalen-1-yl-urea	1-Adamantan-1-yl-3-(3,5-difluoro- 4-hydroxy-phenyl)-urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-phenoxy-phenyl)- urea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-phenyl-urea
HO NA OMA	TZ O TZ		HN OH	HN OH
837	838	839	840	841

331.1	301.2	321.0	335.1	335.3
330.76	300.78	320.77	334.80	334.80
∢	A	¥	¥	· <b>4</b>
C14H19CIN2O5	C14H21CIN2O3	C16H17CIN2O3	C17H19CIN2O3	C17H19CIN2O3
3-{3-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-ureido}-propionic acid ethyl ester	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-pentyl- urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-pentylurea	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-(2- methyl-benzyl)-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-5-(1-phencthyl-urea
HZ OH	HO H	IN OH	HO HO TO	N N N OH
842	843	844	845	846

343.7	287.6	327.5	389.4	376.2
342.86	286.75	326.82	388.77	375.63
¥	¥	¥	¥	. ч
C17H27CI2N2O2	C13H19CIN2O3	C16HZ3CINZO3	C17H16ClF3N2O3	C15H13Cl3N2O3
1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(1,1,3,3-tetramethyl-butyl)-urea	1-tert-Butyl-3-[3-chloro-4- hydroxy-5-(1-hydroxy-ethyl)- phenyl]-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-cyclohexylmethyl-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-benzyl)-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-chloro-phenyl)-urea
IZ O IZ O O	HO TEN OF	E O TIN	HO N N N N N N N N N N N N N N N N N N N	IN OH
847	848	859	850	851

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341.6	375.0	313.0	391.2	332.0
341.19	374.74	312.79	390.74	331.75
<b>V</b>	∢	¥	∢	. <b>V</b>
C15H14Cl2N2O3	C16H14CIF3N2O3	C15H21CIN2O3	C16H14CIF3N2O4	C16H14CIN3O3
1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-(4- chloro-phenyl)-urea	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-(4- trifluoromethyl-phenyl)-urea	1-[3-Chíoro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3- cyclohexyl-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethoxy-phenyl)-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-cyano-phenyl)-urea
P P P P P P P P P P P P P P P P P P P	HO HO LOS	N O HO	HO HO NH OCH	NO N
852	853	854	855	856

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351.1	321.0	337.1	335.2	397.2
350.75	320.77	336.77	334.80	. 396.82
<b>V</b>	∢	∢	∢ .	. <b>4</b>
C16H15CIN2O5	C16H17CIN2O3	C16H17CIN2O4	C17H19CINZO3	C18H21CIN2O6
1-Benzo[1,3]dioxol-5-yl-3-[3- chloro-4-hydroxy-5-(1-hydroxy- ethyl)-phenyl]-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-o-tolylurea	1-[3-Chioro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(3-methoxy-phenyl)-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(2,6-dimethyl-phenyl)-urea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(3,4,5-trimethoxy-phenyl)-urea
F OF OF	F OF	HO H	TZ OF	HO N O O O O O O O O O O O O O O O O O O
857	828	859	098	861

862	HO HO HO	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-naphthalen-1-yl-urea	C19H17CIN2O3	∢	356.80	357.1
863	P - D - D	1-Adamantan-1-yl-3-[3-chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-urea	C19H25CIN2O3	<b>∀</b>	364.87	365.1
864	HO DE TENTO TO TENTO TENTO TO TENTO TEN	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-(4- phenoxy-phenyl)-urea	C21H19CIN2O4	∢	398.84	399.0
865	HO HO TO	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-phenyl- urea	C15H15CINZO3	₹ .	306.74	307.0
998	IZ S TZ S	1-(3-Chloro-4-hydroxy-phenyi)-3- pentyl-thiourea	C12H17CINZOS	П	272.79	272.9

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293.1	306.9	307.1	315.0	258.9	245.0
292.78	306.81	306.81	314.87	258.77	244.74
I	Н	н	I	· <b></b>	I
C14H13CIN2OS	CISH15CIN2OS	C15H15CIN2OS	C15H23CIN2OS	C11H15CINZOS	C10H13CINZOS
1-Benzyl-3-(3-chloro-4-hydroxy- phenyl)-thiourea	1-(3-Chloro-4-hydroxy-phenyl)-3- (2-methyl-benzyl)-thiourea	1-(3-Chloro-4-hydroxy-phenyl)-3- phenethyl-thiourea	1-(3-Chloro-4-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	1-tert-Butyl-3-(3-chloro-4- hydroxy-phenyl)-thiourea	1-(5-Chloro-2-hydroxy-phenyl)-3- isopropyl-thiourea
TZ O	TZ OF	IZ S	TZ OH	IZ S	N S OH
867	898	698	870	871	872

873	IZ IZ	1-(3-Chloro-4-hydroxy-phenyl)-3-cyclohexylmethyl-thiourea	C14H19CIN2OS	П	298.83	299.1
	₽ 	•				
874	JE S IN S I	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	CISH12CIF3N2OS	I	360.78	361.1
875	D TN	1-(3-Chloro-4-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-thiourea	C13H9C13NZOS	I	347.65	347.9
876	HA LA	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-chloro-phenyl)-thiourea	C13H10Cl2N2OS	I	313.20	313.5
877	HZ S TZ S	1-(3-Chloro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	C14H10CIF3N2OS	. ⊷	346.76	347.0
878	12 % 12 % 12 %	1-(3-Chloro-4-hydroxy-phenyl)-3- cyclohexyl-thiourea	C13H17CIN2OS	ü	284.80	285.0

347.0	279.0	307.5	327.4	341.4	341.5
346.76	278.76	307.24	327.23	341.26	341.26
I	<b></b>	ĭ		I	
C14H10CIF3N2OS	C13H11CIN2OS	C12H16C12N2OS	C14H12Cl2N2OS	C15H14Cl2N2OS	C15H14Cl2N2OS
1-(3-Chloro-4-hydroxy-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	1-(3-Chloro-4-hydroxy-phenyl)-3- phenyl-thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-pentyl-thiourea	1-Benzyl-3-(3,5-dichloro-4- hydroxy-phenyl)-thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(2-methyl-benzyl)- thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-phenethyl-thiourea
H S IN S	\$\frac{1}{2} \times 5	D P IZ S S S S S S S S S S S S S S S S S S S	TIN SO TO	TN S TO	D H OH IN
879	088	881	882	883	884

T		T		1-3	
349.6	293.6	279.5	333.5	395.5	382.3
349.32	293.21	279.19	333.28	395.23	382.09
I	I	П	H	н	н
C15H22CI2N2OS	C11H14Cl2N2OS	C10H12Cl2N2OS	C14H18Cl2N2OS	C15H11Cl2F3N2OS	C13H8Cl4N2OS
1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-thiourea	1-tert-Butyl-3-(3,5-dichloro-4- hydroxy-phenyl)-thiourea	1-(5-Chloro-4-hydroxy-phenyl)-3- isopropyl-thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- benzyl)-thiourea	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(3,5-dichloro-phenyl)-thiourea
D TZ S	JZ OF	O OF OF O	D TZ D D D D D D D D D D D D D D D D D D	HO COP3	D TZ S S S S S S S S S S S S S S S S S S
885	988	887	88	888	890

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345.9	381.6	319.6	381.4	313.5	283.9
345.65	381.2	319.25	381.20	313.20	283.35
I	I	П	· I	I .	I
C13H9Cl3N2OS	C14H9Cl2F3N2OS	C13H16Cl2N2OS	C14H9Cl2F3N2OS	C13H10Cl2N2OS	C12H17N3O3S
1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(4-chloro-phenyl)-thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiourea	1-(3,5-Dichloro-4-hydroxy-phenyl)-3-cyclohexyl-thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea	1-(3,5-Dichloro-4-hydroxy- phenyl)-3-phenyl-thiourea	1-(4-Hydroxy-3-nitro-phenyl)-3- pentyl-thiourea
17 % 17 %	D TZ S TZ	IZ O TZ O TZ	IN S TO S	IZ S	IN S IN OH
891	892	893	894	895	968

т		
304.0	317.9	318.0
303.34	317.36	317.36
I	П	ы
C14H13N3O3S	C15H15N3O3S	C15H15N3O3S
1-Benzyl-3-(4-hydroxy-3-nitro- phenyl)-thiourea	1-(4-Hydroxy-3-nitro-phenyl)-3- (2-methyl-benzyl)-thiourea	1-(4-Hydroxy-3-nitro-phenyl)-3- phenethyl-thiourea
HN S HN S S S S S S S S S S S S S S S S	IN NO H	IN NO H
897	868	668

	Structure	Chemical name	Formula	Synthesis methods	MolWeight	MS data
98	HZ SH	1-(4-Hydroxy-3-nitro-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	C15H23N3O3S	I	325.43	326.1
901	N <sub>S</sub> O N <sub>S</sub> O N <sub>S</sub> O N <sub>S</sub> O N <sub>S</sub> O	1-tert-Butyl-3-(4-hydroxy-3-nitro- phenyl)-thiourea	C11H15N3O3S	I	269.32	239.9
902	IN NOO H	1-(4-Hydroxy-3-nitro-phenyl)-3- isopropyl-thiourea	C10H13N3O3S		255.29	255.9
903	IN NO OH	1-Cyclohexylmethyl-3-(4- hydroxy-3-nitro-phenyl)-thiourea	C14H19N3O3S	П	309.38	309.9
904	PAN NA N	1-(4-Hydroxy-3-nitro-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	C15H12F3N3O3S	н	371.33	372.0
905	D HN S HN	1-(3,5-Dichloro-phenyl)-3-(4- hydroxy-3-nitro-phenyl)-thiourea	C13H9Cl2N3O3S	I	358.20	358.6

			r	т		
324.2	357.9	296.0	357.6	289.5	256.8	276.7
323.75	357.31	295.36	357.31	289.31	256.34	276.33
П	I	Ι	H	1	I	н
C13H10CIN3O3S	C14H10F3N3O3S	C13H17N3O3S	C14H10F3N3O3S	C13H11N3O3S	C12H17FN2OS	C14H13FN2OS
1-(4-Chloro-phenyl)-3-(4-hydroxy-3-nitro-phenyl)-thiourea	1-(4-Hydroxy-3-nitro-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	1-Cyclohexyl-3-(4-hydroxy-3- nitro-phenyl)-thiourea	1-(4-Hydroxy-3-nitro-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	1-(4-Hydroxy-3-nitro-phenyl)-3- phenyl-thiourea	1-(3-Fluoro-4-hydroxy-phenyl)-3- pentyl-thiourea	1-Benzyl-3-(3-fluoro-4-hydroxy- phenyl)-thiourea
IN SO I	IZ O	N.CO OH	HO NE OF S	LZ S LZ OH	IN OH	IN DE
906	206	806	606	910	911	912

913	II S	1-(3-Fluoro-4-hydroxy-phenyl)-3- (2-methyl-benzyl)-thiourea	CISH15FN2OS	I	290.36	290.5
914	IN S	1-(3-Fluoro-4-hydroxy-phenyl)-3- phenethyl-thiourea	CISHISFN2OS	I	290.36	290.5
915	H S S S S S S S S S S S S S S S S S S S	1-(3-Fluoro-4-hydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	C15H23FN2OS	Н	298.42	298.7
916	TN SOF	1-tert-Butyl-3-(3-fluoro-4- hydroxy-phenyl)-thiourea	C11H15FN2OS	П	242.31	242.8
917	TN S	1-(3-Fluoro-4-hydroxy-phenyl)-3- isopropyl-thiourea	C10H13FN2OS	· I	228.29	228.5
918	TX of	1-(3-Fluoro-4-hydroxy-phenyl)-3- cyclohexylmethyl-thiourea	C14H19FN2OS	Н	282.38	282.7
919	HO NH S	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-benzyl)- thiourea	C15H12F4N2OS	П	344.33	344.7

331.5	297.1	330.6	268.6	330.5	262.5	254.6
331.19	296.75	330.30	268.35	330.30	262.30	254.35
н	I	I		П	<b>L</b>	I
C13H9Cl2FN2OS	C13H10CIFN2OS	C14H10F4N2OS	C13H17FN2OS	C14H10F4N2OS	C13H11FN2OS	C12H18N2O2S
1-(3-Fluoro-4-hydroxy-phenyl)-3- (3,5-dichloro-phenyl)-thiourea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-chloro-phenyl)-thiourea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (4-trifluoromethyl-phenyl)- thiourea	1-(3-Fluoro-4-hydroxy-phenyl)-3- cyclohexyl-thiourea	1-(3-Fluoro-4-hydroxy-phenyl)-3- (2-trifluoromethyl-phenyl)- thiourea	1-(3-Fluoro-4-hydroxy-phenyl)-3- phenyl-thiourea	1-(2,4-Dihydroxy-phenyl)-3- pentyl-thiourea
TZ SS	TZ S TZ OH	LN N N N N N N N N N N N N N N N N N N	TZ S	H N S	TZ SS	HO H
920	921	922	923	924	925	926

126	HO TIN W	1-Benzyl-3-(2,4-dihydroxy- phenyl)-thiourea	C14H14N2O2S	Ι	274.34	274.7
928	TZ S	1-(2,4-Dihydroxy-phenyl)-3-(2- methyl-benzyl)-thiourea	CISHI6N2O2S	I	288.36	288.6
929	F N S	1-(2,4-Dihydroxy-phenyl)-3- phenethyl-thiourea	C15H16N2O2S	I	288.36	288.6
930	HO SHOW OH	1-(2,4-Dihydroxy-phenyl)-3- (1,1,3,3-tetramethyl-butyl)- thiourea	C15H24N2O2S		296.43	296.7
931	FIZ S	1-tert-Butyl-3-(2,4-dihydroxy- phenyl)-thiourea	C11H16N2O2S	Н	240.32	240.6
932	HZ S	1-(2,4-Dihydroxy-phenyl)-3- isopropyl-thiourea	C10H14N2O2S	I	226.30	226.7
933	FO TEN	1-Cyclohexylmethyl-3-(2,4- dihydroxy-phenyl)-thiourea	C14H20N2O2S	П	280.39	280.7

342.6	329.5	295.0	328.7	266.7	328.6
342.34	329.20	294.76	328.31	266.36	328.31
I	I	1	·	I	Н
C15H13F3N2O2S	C13H10CIZNZO2S	C13H11CIN2O2S	C14H11F3N2O2S	C13H18N2O2S	C14H11F3N2O2S
1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethyl-benzyl)-thiourea	1-(3,5-Dichloro-phenyl)-3-(2,4- dihydroxy-phenyl)-thiourea	1-(4-Chloro-phenyl)-3-(2,4- dihydroxy-phenyl)-thiourea	1-(2,4-Dihydroxy-phenyl)-3-(4- trifluoromethyl-phenyl)-thiourea	1-Cyclohexyl-3-(2,4-dihydroxy-phenyl)-thiourea	1-(2,4-Dihydroxy-phenyl)-3-(2- trifluoromethyl-phenyl)-thiourea
HO OH	TZ S TZ OH	TZ S	HN SO H	IN HOUSE	HO HO S
934	935	936	937	938	939

260.6	396.5	416.4	430.5	430.5	438.6
260.31	396.14	416.13	430.16	430.16	438.22
1	П	H	ы	I	н
C13H12N2O2S	C12H16Br2N2OS	C14H12Br2N2OS	C15H14Br2N2OS	C15H14Br2N2OS	C15H22Br2N2OS
1-(2,4-Dihydroxy-phenyl)-3- phenyl-thiourea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-pentyl-thiourea	1-Benzyl-3-(3,5-dibromo-4- hydroxy-phenyl)-thiourea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(2-methyl-benzyl)- thiourea	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-phenethyl-thiourea	1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-thiourea
IX S	HN PRO TEN	HO HO NEW YORK THE	HN S HN S	HZ S HZ S S S S S S S S S S S S S S S S	TN SO
940	941	942	943	944	945

422.5	422.5	484.5
422.18	422.18	422.18
I	· H	· I I I
C14H18Br2N2OS	C14H18Br2N2OS C15H11Br2F3N2OS	C14H18Br2N2OS C15H11Br2F3N2OS C13H8Br2CI2N2OS
1-(3,5-Dibromo-4-hydroxy-phenyl)-3-cyclohexylmethyl-thiourea		1-(3,5-Dibromo-4-hydroxy-phenyl)-3-cyclohexylmethyl-thiourea 1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(4-trifluoromethyl-benzyl)-thiourea 1-(3,5-Dibromo-4-hydroxy-phenyl)-3-(3,5-dichloro-phenyl)-thiourea
TN T	IZ IZ O	
948	948	949 949 950

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952	HO NH	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiourea	C14H9Br2F3N2OS	Н	470.10	470.6
953	HA S HA S S S S S S S S S S S S S S S S	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-cyclohexyl-thiourea	C13H16Br2N2OS	Н	408.15	408.5
954	HO Br	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea	C14H9Br2F3N2OS		470.10	470.5
955	IN OH	1-(3,5-Dibromo-4-hydroxy- phenyl)-3-phenyl-thiourea	C13H10Br2N2OS	. 1	402.10	402.6
926	HZ S	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-pentyl-thiourea	C12H1GF2N2OS	н	274.33	274.8
957	IZ U	1-Benzyl-3-(3,5-difluoro-4- hydroxy-phenyl)-thiourea	C14H12F2N2OS	Н	294.32	294.7

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308.6	308.6	316.8	260.5	246.5	300.6
308.35	308.35	316.41	260.30	246.28	300.37
Ι	I		Ι	I	П
C15H14F2N2OS	C15H14F2N2OS	C15H22F2N2OS	C11H14F2N2OS	CIOHIZEZNZOS	C14H18F2N2OS
1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(2-methyl-benzyl)- thiourea	1-(3,5-Difluoro-4-hydroxy-phenethyl-thiourea	1-(3,5-Difluoro-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-thiourea	1-tert-Butyl-3-(3,5-Difluoro-4-hydroxy-phenyl)-thiourea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-isopropyl-thiourea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-cyclohexylmethyl- thiourea
TZ S	IZ W	IZ OH	IZ OH	IN SO	IN OH
958	929	096	1961	962	963

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1-(3,5-Difluoro-4-hydroxy-phenyl)-3-(4-trifluoromethyl-benzyl)-thiourea	1-(3,5-Difluoro- phenyl)-3-(4-tri- benzyl)-thioure:	4-hydroxy- fluoromethyl-	CISH11FSN2OS	Ι	362.32	362.8
1-(3,5-Diffuo phenyl)-3-(3,	1-(3,5-Difluo phenyl)-3-(3, thiourea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(3,5-dichloro-phenyl)- thiourea	C13H8C12F2N2OS	H	349.18	349.7
FY HO THE STATE I - (3,5-Diffu phenyl)-3-(4 thiourea	1-(3,5-Diffu phenyl)-3-(4 thiourea	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-chloro-phenyl)- thiourea	C13H9CIF2N2OS		314.74	315.2
1-(3,5-Difluoro-ces phenyl)-3-(4-trifl phenyl)-thiourea	1-(3,5-Diffu phenyl)-3-( phenyl)-thi	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(4-trifluoromethyl- phenyl)-thiowea	C14H9F5NZOS	I	348.29	348.8
HO S Phenyl)-3	1-(3,5-Dif phenyl)-3	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-cyclohexyl-thiourea	C13H16F2N2OS	I	286.34	286.6
F H CF3 1-(3,5-Difluoro-4 phenyl)-3-(2-trifl phenyl)-thiourea	1-(3,5-Dif phenyl)-3- phenyl)-th	1-(3,5-Difluoro-4-hydroxy- phenyl)-3-(2-trifluoromethyl- phenyl)-thiourea	C14H9F5N2OS	н	348.29	348.8

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280.5	316.9	337.2	351.1	. 351.0
280.29	316.85	336.84	350.86	350.86
Ι	m	· H	<b>1</b>	1
C13H10F2N2OS	C14H21CIN2O2S	C16H17CIN2O2S	C17H19CIN2O2S	C17H19CIN2O2S
1-(3,5-Difluoro-4-hydroxy- phenyl)-3-phenyl-thiourea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-pentyl-thiourea	1-Benzyl-3-[3-chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-thiourea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(2-methyl-benzyl)-thiourea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-phenethyl-thiourea
TZ SS	OH N N N	IN DA	TN OF	FINAL STATE OF THE
970	971	972	973	974

359.2	303.0	289.0	343.1	405.2
358.93	302.82	288.79	342.88	404.83
Н	ы	·	H	I
C17H27CIN2O2S	C13H19CIN2O2S	C12H17CIN2O2S	C16H23CIN2O2S	CI7H16CIF3N2O2S
1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-(1,1,3,3- tetramethyl-butyl)-thiourea	1-tert-Butyl-3-[3-chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-thiourea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-isopropyl-thiourea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-cyclohexylmethyl-thiourea	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-benzyl)-thiourea
HO HO TO	HO OH DING TO THE OH TH	HO TEN STATE OF THE STATE OF TH	F. S.	HN HN S
975	976	77.6	978	979

086	HO TO	1-[3-Chloro-4-hydroxy-5-(1- hydroxy-ethyl)-phenyl]-3-(3,5- dichloro-phenyl)-thiourea	C15H13Cl3N2O2S	I	391.70	392.0
981	IN S POP POP POP POP POP POP POP POP POP P	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-chloro-phenyl)-thiourea	CISH14CI2N2O2S	Ι	357.25	357.6
982	HO H	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(4-trifluoromethyl-phenyl)-thiourea	C16H14CIF3N2O2S	I	390.81	391.0
983	HO OH SO TO	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-cyclohexyl-thiourea	C15H21CIN2O2S	I	328.86	329.4
984	HO H	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-(2-trifluoromethyl-phenyl)-thiourea	C16H14CIF3N2O2S	1	390.81	391.0

985	HO OH OH OH	1-[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl)-phenyl]-3-phenylthiourea	CI5H15CIN2O2S	I	322.81	323.1
986	TZ OH	2-Chloro-4-(2-phenylsulfanyl- benzylamino)-phenol	C19H16CINOS	Q	341.85	342.2
786	TZ OF	2-Chloro-4-(2-p-tolylsulfanyl- benzylamino)-phenol	C20H18CINOS	Д	355.88	356.3
886	IN DE	2-Chloro-4-[2-(4-chloro- phenylsulfanyl)-benzylamino]- phenol	C19H15CIZNOS	Q	376.30	376.8
686	HON IS	2-Chloro-4-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol	C19H15CINZO3S	Ω	386.85	387.2

372.4	376.8	376.8	411.2	399.3
371.88	376.30	376.30	410.74	398.91
D	Q	Q	Ω	Q
C20H18CINO2S	C19H15CIZNOS	C19H15Cl2NOS	C19H14CI3NOS	C21H19CINZO2S
2-Chloro-4-[2-(4-methoxy-phenyll-benzylamino]-phenol	2-Chloro-4-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Chloro-4-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Chloro-4-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(3-Chloro-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
LN IN	TZ O	DE TOUR DE TOU	TZ 5	HO CO
066	991	365	993	994

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393.4	421.7	401.2	391.9
392.90	421.30	400.88	391.31
D	D	D	Q
C22H17CINZOS	C19H14Cl2N2O3S	C20H17CIN2O3S	C19H16Cl2N2OS
2-Chloro 4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	2-Chloro-4-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2-Chloro-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2-chloro-phenol
Z D D D	ON TEX	ON THE TOTAL	HO D D D D
995	966	266	866

408.7	376.7	390.7	411.1	421.8
408.30	376.30	390.33	410.75	421.30
D	D	Q	Q	<b>Q</b>
C19H15Cizno3S	C19H15CIZNOS	C20H17CIZNOS	C19H14CI3NOS	C19H14CI2N2O3S
2-Chloro-4-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol	2,6-Dichloro-4-(2-phenylsulfanyl- benzylamino)-phenol	2,6-Dichloro-4-(2-p-tolylsulfanyl- benzylamino)-phenol	2,6-Dichloro-4-[2-(4-chloro-phenylsulfanyl)-benzylamino]-phenol	2,6-Dichloro-4-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol
	TZ OF	D P	D D D	SON POPULATION OF THE POPULATI
666	1000	1001	1002	1003

5.7	1.2	1.2	445.6	433.8
406.7	411.2	411.2	44.	43.
406.33	410.75	410.75	445.19	433.36
Q	D	Q	Q	α .
C20H17CIZNO2S	C19H14Cl3NOS	C19H14CI3NOS	C19H13Cl4NOS	C21H18CIZN2O2S
2,6-Dichloro-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	2,6-Dichloro-4-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2,6-Dichloro-4-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2,6-Dichloro-4-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(3,5-Dichloro-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-
HO CI	TIN DO DE	HO S C C C C C C C C C C C C C C C C C C	H D D D D D D D D D D D D D D D D D D D	TZ S
1004	1005	1006	1007	1008

427.8	456.0	435.7	426.0
427.35	455.74	435.33	425.76
Q	Q	Q	Q
C22H16CI2N2OS	C19H13CI3N2O3S	C20H16Cl2N2O3S	C19H15Cl3N2OS
2,6-Dichloro-4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	2,6-Dichloro-4-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2,6-Dichloro-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-2,6- dichloro-phenol
HO D D D D D D D D D D D D D D D D D D D	D H O H	CC NO S NO	THE SOUTH OF THE S
1009	1010	1011	1012

443.1	352.8	366.8	387.2	397.7
442.75	352.41	366.43	386.85	397.40
Q	Q	Q	Q	Q
C19H14Cl3NO3S	C19H16N2O3S	C20H18N2O3S	C19H15CIN2O3S	C19H15N3OSS
2,6-Dichloro-4-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol	2-Nitro-4-(2-phenylsulfanyl- benzylamino)-phenol	2-Nitro-4-(2-p-tolylsulfanyl- benzylamino)-phenol	4-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2-nitro-phenol	2-Nitro-4-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol
HO CI	O <sub>2</sub> N N O <sub>2</sub> O	O <sub>2</sub> N HO	OH N <sub>2</sub> OO	NO <sub>2</sub> O <sub>N</sub> O <sub>2</sub> O <sub>2</sub> O <sub>3</sub> O <sub>3</sub> O <sub>4</sub> O <sub>3</sub> O <sub>4</sub> O <sub>5</sub>
1013	1014	1015	1016	1017

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382.8	387.2	387.1	421.7	409.9
382.43	386.85	386.85	421.30	409.46
Ω	Q	Q	Q	Q
C20H18N2O4S	C19H15CIN2O3S	C19H15CIN2O3S	C19H14Cl2N2O3S	C21H19N3O4S
4-[2-(4-Methoxy-phenylsulfanyl)- benzylamino]-2-nitro-phenol	4-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-2-nitro-phenol	4-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-2-nitro-phenol	4-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2- nitro-phenol	N-(4-{2-[(4-Hydroxy-3-nitro-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
O <sub>2</sub> N (1) O <sub>MB</sub>	HO NEO	N <sub>2</sub> O <sub>2</sub> N H	N <sub>c</sub> O <sub>O</sub>	O <sub>2</sub> N H
1018	1019	1020	1021	1022

403.8	432.2	411.9	444.3
403.45	431.85	411.43	443.90
Ð	Q	Д	Q
C22H17N3O3S	C19H14CIN3O5S	C20H17N3O5S	C21H18ClN3O4S
2-Nitro-4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	4-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2-nitro-phenol	2-Nitro-4-(5-nitro-2-p- tolylsulfanyl-benzylamino)-phenol	N-{4-(4-Chloro-phenylsulfanyl)-3- [(4-hydroxy-3-nitro-phenylamino)- methyl]-phenyl}-acetamide
O <sub>2</sub> N K	ON H NGO	N <sub>2</sub> ON N <sub>2</sub> OH	O <sub>2</sub> N H S
1023	1024	1025	1026

419.2	324.6	340.8	360.1	370.8
418.85	325.40	339.43	359.84	370.40
Q	. Д	. Q	Q	Q
C19H15CIN2O5S	C19H16FNOS	C20H18FNOS	C19H15CIFNOS	C19H15FN2O3S
4-[2-(4-Chloro-benzenesulfonyl)-benzylamino]-2-nitro-phenol	2-Fluoro-4-(2-phenylsulfanyl- benzylamino)-phenol	2-Fluoro-4-(2-p-tolylsulfanyl- benzylamino)-phenol	2-Fluoro-4-[2-(4-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-4-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol
D N <sup>2</sup> O N <sup>2</sup> O	PL S S S S S S S S S S S S S S S S S S S	THE STATE OF THE S	TZ, Q	TIN ON
1027	1028	1029	1030	1031

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355.8	360.2	360.3	394.6	382.9
355.43	359.84	359.84	394.29	382.45
А	Q	Q	Q	Q
C20H18FNO2S	C19H15CIFNOS	C19H15CIFNOS	C19H14Cl2FNOS	C21H19FN2O2S
2-Fluoro-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-4-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2-Fluoro-4-[2-(3-chloro- phenylsulfanyl)-benzylamino]- phenol	2-Fluoro-4-[2-(3,4-dichloro- phenylsulfanyl)-benzylamino]- phenol	N-(4-{2-[(3-Fluoro-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
HO S COME	HO N N N N N N N N N N N N N N N N N N N	HO S COI	HO N	HO S S NHAC
1032	1033	1034	1035	1036

377.0	405.3	384.9	375.1
376.45	404.84	384.42	374.86
Д	D	D	D
C22H17FN2OS	C19H14CIFN2O3S	C20H17FN2O3S	C19H16CIFN2OS
2-Fluoro-4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	2-Fluoro-4-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2-Fluoro-4-(5-nitro-2-p- tolyisulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-2- fluoro-phenol
HZ OH	HO S CI	HO S	Z-IN NO H
1037	1038	1039	1040

	7-65			<del></del>
392.0	323.8	337.8	358.2	368.7
391.84	323.41	337.44	357.85	368.41
A	Q	Q	Q	Q
C19H15CIFNO3S	C19H17NO2S	C20H19NO2S	C19H16CINO2S	C19H16N2O4S
2-Fluoro-4-[2-(4-chloro-benzenesulfonyl)-benzylamino]-phenol	4-(2-Phenylsulfanyl-benzylamino)- benzene-1,3-diol	4-(2-p-Tolylsulfanyl- benzylamino)-benzene-1,3-diol	4-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-benzene-1,3-diol	4-[2-(4-Nitro-phenylsulfanyl)- benzylamino]-benzene-1,3-diol
HO O <sub>2</sub> S	HO CH K	HO S	HO NO	HO S NO2
1041	1042	1043	1044	1045

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353.7	358.3	358.1	392.7	380.8
353.43	357.85	357.86	392.30	380.46
Ð	Q	Q	Q	Q
C20H19NO3S	C19H16CINO2S	C19H16CINO2S	C19H15Cl2NO2S	C21H20N2O3S
4-[2-(4-Methoxy-phenylsulfanyl)- benzylamino]-benzene-1,3-diol	4-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-benzene-1,3-diol	4-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-benzene-1,3-diol	4-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]- benzene-1,3-diol	N-(4-{2-[(2,4-Dihydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
HO S ONB	HO S S	HO OH NO S	HO S S	HO CH NHAC
1046	1047	1048	1049	1050

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374.9	403.2	382.7	373.0
374.46	402.85	382.43	372.87
D	D	Q	Q
C22H18N2O2S	C19H15CINZO4S	C20H18NZO4S	C19H17CIN2O2S
4-[2-(Quinolin-7-ylsulfanyl)-benzylamino]-benzenc-1,3-diol	4-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-benzene-1,3- diol	4-(5-Nitro-2-p-tolylsulfanyl- benzylamino)-benzene-1,3-diol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-benzene-1,3-diol
1	P ON OH	PON	HN NO OH
1051	1052	1053	1054

4-[2-(4-Ch benzylamii	4-[2-(4-Chloro-benzenesulfonyl)- benzylamino]-benzene-1,3-diol	C19H16CINO4S	Ω	389.85	390.2
2,6-Dibro benzylam	2,6-Dibromo-4-(2-phenylsulfanyl-benzylamino)-phenol	C19H15Br2NOS	Q	465.20	465.7
2,6-Dibro benzylam	2,6-Dibromo-4-(2-p-tolylsulfanyl-benzylamino)-phenol	C20H17Br2NOS	Q	479.23	479.3
2,6-Dibra phenylsu phenol	2,6-Dibromo-4-[2-(4-chloro-phenylsulfanyl)-benzylamino]- C19H14	C19H14Br2CINOS	D	499.65	500.1
2,6-Dibre phenylsu phenol	2,6-Dibromo-4-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol	C19H14Br2N2O3S	D	510.2	510.1

495.3	499.8	499.8	534.2	522.4
495.23	499.65	499.65	534.09	522.25
Q	D	Q	Q	Q
C20H17B/2NO2S	C19H14Br2CINOS	C19H14Br2CINOS	C19H13Br2Cl2NOS	C21H18Br2N2O2S
2,6-Dibromo-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	2,6-Dibromo-4-[2-(2-chloro-phenylsulfanyl)-benzylamino]-phenol	2,6-Dibromo-4-[2-(3-chloro-phenylsulfanyl)-benzylamino]-phenol	2,6-Dibromo-4-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-phenol	N-(4-{2-[(3,5-Dibromo-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
HO S S S S S S S S S S S S S S S S S S S	HA PART OF THE PAR	DH NO	D D D	HO S S NIHAe
1360	1061	1062	1063	1064

516.4	544.8	524.6	514.9
516.25	544.64	524.23	514.66
Q	D	Q	Ð
C22H16Br2N2OS	C19H13Br2CIN2O3 S	C20H16Br2N2O3S	C19H15Br2CIN2OS
2,6-Dibromo-4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	2,6-Dibromo-4-[2-(4-chloro- phenylsulfanyl)-5-nitro- benzylamino]-phenol	2,6-Dibromo-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2,6-dibromo-phenol
TZ S S S S S S S S S S S S S S S S S S S	N N N N N N N N N N N N N N N N N N N	DON DE LES	HO S S S S S S S S S S S S S S S S S S S
1065	1066	1067	1068

373.7	378.1	378.2	412.6	400.8
373.42	377.83	377.83	412.28	400.44
D	D	D	Q	Q
C20H17F2NO2S	C19H14CIF2NOS	C19H14CIF2NOS	C19H13Cl2F2NOS	C21H18F2N2O2S
2,6-Difluoro-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	4-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-2,6-difluoro-phenol	4-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-2,6-difluoro-phenol	4-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2,6- difluoro-phenol	N-(4-{2-[(3,5-Difluoro-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl}-acetamide
TZ S TZ S S S S S S S S S S S S S S S S	TZ OF	TIN OF THE STATE O	TZ S	TZ OH
1074	1075	1076	1077	1078

394.9	423.3	402.8	393.0
394.44	422.83	402.41	392.85
D	Д	Q	Q
C22H16F2N2OS	C19H13CIF2N2O3S	C20H16F2N2O3S	C19H15CIFZN2OS
2,6-Difluoro-4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	4-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2,6-difluoro- phenol	2,6-Difluoro-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2,6-difluoro-phenol
	DE LES	N N N N N N N N N N N N N N N N N N N	HZ SS
1079	1080	1081	1082

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392.3	342.3	400.2	420.9	431.3
391.84	341.85	399.93	420.35	430.90
. О	D	Q	Ω	Q
C19H14CIF2NO3S	C21H20CINO2S	C22H22CINO2S	C21H19Cl2NO2S	C21H19CIN2O4S
4-[2-(4-Chloro-benzenesulfonyl)-benzylamino]-2,6-difluoro-phenol	2-Chloro-6-(1-hydroxy-ethyl)-4- (2-phenylsulfanyl-benzylamino)- phenol	2-Chloro-6-(1-hydroxy-ethyl)-4- (2-p-tolylsulfanyl-benzylamino)- phenol	2-Chloro-4-[2-(4-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	2-Chloro-6-(1-hydroxy-ethyl)-4- [2-(4-nitro-phenylsulfanyl)- benzylamino]-phenol
TN NT N	5 - 9 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 -	F D D T	TZ S	FON DE SON
1083	1084	1085	1086	1087

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1088	HO S S S S S S S S S S S S S S S S S S S	2-Chloro-6-(1-hydroxy-ethyl)-4- [2-(4-methoxy-phenylsulfanyl)- benzylamino]-phenol	C22H22CINO3S	Д	415.93	416.3
1089	# O P	2-Chloro-4-[2-(2-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	C21H19Cl2NO2S	Д	420.35	420.9
1090	E S S S S S S S S S S S S S S S S S S S	2-Chloro-4-[2-(3-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-eftyl)-phenol	C21H19ClZNO2S	·	420.35	420.8
1091	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	2-Chloro-4-[2-(3,4-dichloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	C21H18Cl3NO2S	Ω	454.80	455.2
1092	HO NHAC	N-[4-(2-[[3-Chloro-4-hydroxy-5-(1-hydroxy-ethyl]-phenylamino]-acetamide	C23H23CIN2O3S	Q	442.96	443.4

437.3	465.9	445.3	435.6
436.95	465.35	444.93	435.37
D	D	Q	Д
C24H21CIN2O2S	C21H18CI2N2O4S	C22H21CIN2O4S	C21H20Cl2N2O2S
2-Chloro-6-(1-hydroxy-ethyl)-4- [2-(quinolin-7-ylsulfanyl)- benzylamino]-phenol	2-Chloro-4-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-6-(1-hydroxy-ethyl)-phenol	2-Chloro-4-(1-hydroxy-ethyl)-6- (5-nitro-2-p-tolylsulfanyl- benzylamino)-phenol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2-chloro-6-(1-hydroxy-ethyl)-phenol
HZ PO TO	S P P P	DY DY DY	HO OH OF OH
1093	1094	1095	1096

452.5	337.8	351.8	371.9	382.7
452.35	337.44	351.46	371.88	382.43
D	D	Q	Q	Q
C21H19Cl2NO4S	C20H19NO2S	C21H21NO2S	C20H18CINO2S	C20H18N2O4S
2-Chloro-4-[2-(4-chloro-benzenesulfonyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol	2-Hydroxymethyl-4-(2- phenylsulfanyl-benzylamino)- phenol	2-Hydroxymethyl-4-(2-p-tolylsulfanyl-benzylamino)-phenol	4-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxymethyl- phenol	2-Hydroxymethyl-4-[2-(4-nitro- phenylsulfanyl)-benzylamino]- phenol
P Of	HO OH	P S S	4 N	HO S NOS
1097	1098	1099	1100	1101

367.9	371.9	371.9	406.5	349.9
367.46	371.88	371.88	406.33	394.49
D	D	Q	Q	Ω
C21H21NO3S	C20H18CINO2S	C20H18CINO2S	C20H17Cl2NO2S	C22H22N2O3S
2-Hydroxymethyl-4-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenol	4-[2-(2-Chloro-phenylsulfanyl)-benzylamino]-2-hydroxymethyl-phenol	4-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxymethyl- phenol	4-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2- hydroxymethyl-phenol	N-(4-{2-[(4-Hydroxy-3-hydroxymethyl-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
HO OH	F 0	TZ OF	D D D	TZ S
1102	1103	1104	1105	1106

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			-
388.8	417.2	396.8	387.1
388.48	416.88	396.46	386.90
D	D	Q	Q
CZ3HZ0NZOZS	C20H17CIN2O4S	C21H20N2O4S	C20H19CIN2O2S
2-Hydroxymethyl-4-[2-(quinolin-7-ylsulfanyl)-benzylamino]-phenol	4-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2- hydroxymethyl-phenol	2-Hydroxymethyl-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2-hydroxymethyl-phenol
TZ OF	PO OH	P P P	FO OH
1107	1108	1109	1110

1111	E S	4-[2-(4-Chloro-benzenesulfonyl)-benzylamino]-2-hydroxymethyl-	C20H18CINO4S	D	403.88	0.44
		phenol				
1112		1-[3-Chloro-2-hydroxy-5-(2-phenylsulfanyl-benzylamino)-phenyl]-ethanone	C21H18CINO2S	D	383.89	384.2
1113		1-[3-Chloro-2-hydroxy-5-(2-p-tolylsulfanyl-benzylamino)-phenyl]-ethanone	C22H20CINO2S	D	397.92	398.2
1114	TZ O	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	C21H17Cl2NO2S	Q	418.34	418.8
1115	O OH OH	1-{3-Chloro-2-hydroxy-5-[2-(4- nitro-phenylsulfanyl)- benzylamino]-phenyl}-ethanone	C21H17CIN2O4S	Ω	428.89	429.3

		<del></del>		
414.5	418.6	418.5	453.0	441.2
413.92	418.34	418.34	452.78	440.94
D	D	D	D	Q
C22H20CINO3S	C21H17G2NO2S	C21H17G2NO2S	C21H16CI3NO2S	C23H21CIN2O3S
1-{3-Chloro-2-hydroxy-5-[2-(4-methoxy-phenylsulfanyl)-benzylamino]-phenyl}-ethanone	1-{3-Chloro-5-[2-(2-chloro-phenylsulfanyl)-benzylamino}-2-hydroxy-phenyl}-ethanone	1-{3-Chloro-5-{2-(3-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	1-{3-Chloro-5-{2-(3,4-dichloro-phenylsulfanyl}-benzylamino]-2-hydroxy-phenyl}-ethanone	N-(4-{2-[(3-Acetyl-5-chloro-4-hydroxy-phenylamino)-methyl]-phenylsulfanyl}-phenyl)-acetamide
Hooms S		D P P P P P P P P P P P P P P P P P P P	FO COL	HO CI S NHAC
1116	1117	1118	1119	1120

435.2	463.7	443.2	433.6
434.94	463.33	442.92	433.35
D	Q	. Д	Q
C24H19CIN2O2S	C21H16Cl2N2O4S	C22H19CIN2O4S	C21H18Cl2N2O2S
1-{3-Chloro-2-hydroxy-5-[2-(quinolin-7-ylsulfanyl)-benzylamino]-phenyl}-ethanone	1-{3-Chloro-5-[2-(4-chloro-phenylsulfanyl)-5-nitro-benzylamino]-2-hydroxy-phenyl}-ethanone	1-[3-Chloro-2-hydroxy-5-(5-nitro- 2-p-tolylsulfanyl-benzylamino)- phenyl]-ethanone	1-{5-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-3-chloro-2-hydroxy-phenyl}-ethanone
TZ O	DE D		D TN D D D D D D D D D D D D D
1121	1122	1123	1124

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1125	D S S S S S S S S S S S S S S S S S S S	1-{3-Chloro-5-[2-(4-chloro-benzenesulfonyl)-benzylamino]-2-hydroxy-phenyl}-ethanone	C21H17Cl2NO4S	D	450.33	450.5
1126	HOOOC N	2-Hydroxy-5-(2-phenylsulfanyl- benzylamino)-benżoic acid	C20H17NO3S	D	351.42	351.6
1127	HOOC N S S	2-Hydroxy-5-(2-p-tolylsulfanyl- benzylamino)-benzoic acid	C21H19NO3S	Q	365.44	365.8
1128	HOOC N N	5-[2-(4-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxy-benzoic acid	C20H16CINO3S	Ω	385.86	385.1
1129	HOOC	2-Hydroxy-5-[2-(4-nitro- phenylsulfanyl)-benzylamino]- benzoic acid	C20H16N2O5S	Q	396.11	396.4

381.6	386.0	386.0	420.7	408.7
381.44	385.86	385.86	420.31	408.47
D	D	Ω	Ω	Д
C21H19NO4S	C20H16CINO3S	C20H16CINO3S	C20H15Cl2NO3S	
2-Hydroxy-5-[2-(4-methoxy- phenylsulfanyl)-benzylamino}- benzoic acid	5-[2-(2-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxy-benzoic acid	5-[2-(3-Chloro-phenylsulfanyl)- benzylamino]-2-hydroxy-benzoic acid	5-[2-(3,4-Dichloro- phenylsulfanyl)-benzylamino]-2- hydroxy-benzoic acid	5-[2-(4-Acetylamino-phenylsulfanyl)-benzylamino]-2-hydroxy-benzoic acid
HOOC N	HOOCH HOOCH	HODG NAME OF THE PARTY OF THE P	HOOC N	HOOC
1130	1131	1132	1133	1134

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402.8	430.9	410.7	387.2
402.46	430.86	410.44	386.90
D	D	. Д	Q
C23H18N2O3S	C20H15CIN2O5S	C21H18N2O5S	C20H19CIN2O2S
2-Hydroxy-5-[2-(quinolin-7- ylsulfanyl)-benzylamino]-benzoic acid	5-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2-hydroxy- benzoic acid	2-Hydroxy-5-(5-nitro-2-p-tolylsulfanyl-benzylamino)-benzoic acid	5-[5-Amino-2-(4-chloro- phenylsulfanyl)-benzylamino]-2- hydroxymethyl-phenol
HOOCC	HNOOH .	HOOC N	HOOCC NAMES OF THE PARTY OF THE
1135	1136	1137	1138

404.1	370.8	384.9	405.0	415.8
403.88	370.40	384.43	404.84	415.40
Q	D	Q	Q	Q
C20H16CINO5S	C19H15FN2O3S	C20H17FN2O3S	C19H14ClFN2O3S	C19H14FN3O5S
5-[2-(4-Chloro-benzenesulfonyl)-benzylamino]-2-hydroxy-benzoic acid	2-Fluoro-6-nitro-4-(2- phenylsulfanyl-benzylamino)- phenol	2-Fluoro-6-nitro-4-(2-p-tolylsulfanyl-benzylamino)-phenol	4-[2-(4-Chloro-phenylsulfanyl)-benzylamino]-2-fluoro-6-nitro-phenol	2-Fluoro-6-nitro-4-[2-(4-nitro-phenylsulfanyl)-benzylamino]-phenol
HOOCC N Op. S. Co.	TX OY	EN SON SON SON SON SON SON SON SON SON SO	HZ ON	HO22N
1139	1140	1141	1142	1143

HONOR HAS COING Phenol	2-Fluoro-4- phenylsulfa nitro-pheno 4-[2-(2-Chl benzylamin phenol 4-[2-(3-Chl benzylamin phenol	2-(4-methoxy- yl)-benzylamino]-6- ro-phenylsulfanyl)- ro-phenylsulfanyl)- ol-2-fluoro-6-nitro- ol-2-fluoro-6-nitro-	C20H17FN2O4S C19H14CIFN2O3S C19H14CIFN2O3S	Q Q	404.84	405.0
IN SON	ō ō	4-[2-(3,4-Dichloro-phenylsulfanyl)-benzylamino]-2-fluoro-6-nitro-phenol	C19H13Cl2FN2O3S	D	439.29	439.9
HN CON	NHAC	N-(4-{2-[(3-Fluoro-4-hydroxy-5- nitro-phenylamino)-methyl]- phenylsulfanyl}-phenyl)- acetamide	C21H18FN3O4S		427.45	427.9

421.6	450.1	429.8	420.2
421.45	449.84	429.42	419.86
Д	Д	Q	Q
C22H16FN3O3S	C19H13CIFN3O5S	C20H16FN3O4S	C19H15CIFN3O2S
2-Fluoro-6-nitro-4-[2-(quinolin-7- ylsulfanyl)-benzylamino]-phenol	4-[2-(4-Chloro-phenylsulfanyl)-5- nitro-benzylamino]-2-fluoro-6- nitro-phenol	2-Fluoro-6-nitro-4-(5-nitro-2-p-tolylsulfanyl-benzylamino)-phenol	4-[5-Amino-2-(4-chloro-phenylsulfanyl)-benzylamino]-2-fluoro-6-nitro-phenol
S SON SON		HO NO S	HZ NON S S S S S S S S S S S S S S S S S S
1149	1150	1151	1152

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437.1	360.5	395.0	416.8
436.84	360.23	394.68	416.34
D	Q		Q
C19H15CIFN2O5S	C19H15Cl2NO2	C19H15Cl3NO2	C23H23Cl2NO2
4-[2-(4-Chloro-benzenesulfonyl)-benzylamino]-2-fluoro-6-nitro-phenol	2,6-Dichloro-4-(3-phenoxy-benzylamino)-phenol	2,6-Dichloro-4-[3-(4-chloro-phenoxy)-benzylamino]-phenol	4-[3-(4-text-Butyl-phenoxy)- benzylamino]-2,6-dichloro-phenol
HON NO.20	TZ OF	5 5 5	TZ 5
1153	1154	1155	1156

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1157	TZ O	4-(3-Benzyloxy-benzylamino)-2,6- dichloro-phenol	C20H17Cl2NO2	Q	374.26	374.6
1158	TZ 5	4-(2-Benzyloxy-benzylamino)-2,6-dichloro-phenol	C20H17CI2NO2	D	374.26	374.6
1159	D D D D D D D D D D D D D D D D D D D	2,6-Dichloro-4-[(naphthalen-1- ylmethyl)-amino]-phenol	C17H13Cl2NO	D	318.20	318.6
1160	TZ OT	2,6-Dichloro-4-(4-methylsulfanyl- benzylamino)-phenol	C14H13Cl2NOS	Ω	314.23	314.7
1161		2,6-Dichloro-4-(2-ethylsulfanyl- benzylamino)-phenol	C15H15Cl2NOS	D	328.26	328.6

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353.6	416.9	334.6	353.4	390.6
353.24	416.77	334.20	353.06	390.26
Q	D	. О	Q	. <b>Q</b>
C17H18Cl2N2O2	C17H12Cl3NOS2	C16H13CI2N3O	C11H8BrCl2NOS	C20H17Cl2NO3
2,6-Dichloro-4-(2-morpholin-4-yl- benzylamino)-phenol	2,6-Dichloro-4-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	2,6-Dichloro-4-[(5-phenyl-2H-imidazol-4-ylmethyl)-amino]-	4-[(5-Bromo-thiophen-2- ylmethyl)-amino]-2,6-dichloro- phenol	2,6-Dichloro-4-[3-(4-methoxy-phenoxy)-benzylamino]-phenol
-z>	D D D D D D D D D D D D D D D D D D D	TV DY	HO CI	
1162	1163	1164	1165	1166

	4	2	∞	ω <sub>ρ</sub>	Ε.
	282.4	336.5	320.8	307.8	342.1
	282.17	336.14	320.57	307.34	341.79
	282	336	320	30	<u>&amp;</u>
	Δ	Q	Д	Q	Q
	· O	F3NO	ON	3	403
	C14H13CIZNO	C14H10CIZF3NO	C13H9Cl3FNO	C19H17NO3	C19H16CINO3
	Ü			Ö	
-	· Iyl-	2,6-Dichloro-4-(3-trifluoromethyl- benzylamino)-phenol	2,6-Dichloro-6-(2-chloro-6-fluoro- benzylamino)-phenol	mino)-	4-[3-(4-Chloro-phenoxy)- benzylamino]-benzene-1,3-diol
	2,6-Dichloro-4-(3-methyl-benzylamino)-phenol	4-(3-trifl)	6-(2-chlc	4-(3-Phenoxy-benzylamino)- benzene-1,3-diol	4-[3-(4-Chloro-phenoxy)-benzylamino]-benzylame-1,
	2,6-Dichloro-4-(3-me benzylamino)-phenol	2,6-Dichloro-4-(3-trif benzylamino)-phenol	2,6-Dichloro-6-(2-chl benzylamino)-phenol	4-(3-Phenoxy-berbenzene-1,3-diol	-(4-Chlorylamino)
	2,6-D	2,6-L	2,6-I	4-(3-	4-[3.
		<b>1 1 1 1 1 1 1 1 1 1</b>	7-5		
	-5	TZ		₹ ĕ	g—
	2 P	5 2	<b>É</b> à	£	Đ.
	1167	1168	1169	1170	1171

1172 Ho Ho Ho Ho Ho Ho Horare Li 3-diol		-					
How the temporal and th	1172	5— Q	4-[3-(4-tert-Butyl-phenoxy)- benzylamino]-benzene-1,3-diol	C23H25NO3	· Q	363.45	363.9
HOOMER A (2-Benzyloxy-benzylamino) C20H19NO3 D 321.37  HOOMER A (1-Benzyloxy-benzylamino) C20H19NO3 D 265.31  HOOMER A (1-Benzyloxy-benzylamino) C17H15NO2 D 265.31  HOOMER A (1-Benzyloxy-benzylamino) C17H15NO2 D 265.31  D 261.34	1173	FIN HOUSE		C20H19NO3	Q	321.37	321.6
4-[(Naphthalen-1-ylmethyl)- C17H15NO2 D 265.31 amino]-benzene-1,3-diol c14H15NO2S D 261.34	1174	HO OH	4-(2-Benzyloxy-benzylamino)- benzene-1,3-diol	C20H19NO3		321.37	321.5
4-(4-Methylsulfanyl-benzene-1,3-diol benzylamino)-benzene-1,3-diol	1175		4-[(Naphthalen-1-ylmethyl)- amino]-benzene-1,3-diol	C17H15NO2	D	265.31	. 265.7
	1176	E E	4-(4-Methylsulfanyl- benzylamino)-benzene-1,3-diol	C14H15NO2S	Q	261.34	261.7

275.9	300.8	364.1	281.6	367.4
275.37	300.35	363.88	281.31	367.09
Q	Д	D	D	Q
CISHI7NO2S	C17H20N2O3	C17H14CINO2S2	C16H15N3O2	C12H10BrC12NOS
4-(2-Ethylsulfanyl-benzylamino)- benzene-1,3-diol	4-(2-Morpholin-4-yl- benzylamino)-benzene-1,3-diol	4-{[2-(4-Chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-benzene-1,3-diol	4-[(5-Phenyl-2H-imidazol-4- ylmethyl)-amino]-benzene-1,3-diol	2-[(5-Bromo-thiophen-2- ylmethyl)-amino]-4,6-dichloro-3- methyl-phenol
F. S.	TIN TO THE TIME TO	S S S S S S S S S S S S S S S S S S S	N HO OH	2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -
1177	1178	1179	1180	1181

		r		
337.8	229.6	283.6	268.0	326.1
337.37	229.27	283.25	267.68	325.79
D	D	D	D	Q
C20H19NO4	C14H15NO2	C14H12F3NO2	C13H11CIFNO2	C19H16CINO2
4-[3-(4-Methoxy-phenoxy)- benzylamino]-benzene-1,3-diol	4-(3-Methyl-benzylamino)- benzene-1,3-diol	4-(3-Trifluoromethyl-benzylamino)-benzene-1,3-diol	4-(2-Chloro-6-fluoro- benzylamino)-benzene-1,3-diol	2-Chloro-4-(3-phenoxy-benzylamino)-phenol
E O O	5—————————————————————————————————————	12 12 15 15	5 TZ	TX QH
1182	1183	1184	1185	1186

360.6	382.2	340.1	340.1
360.23	381.90	339.82	339.82
О	D	Q	Q
C19H15CIZNO2	C23H24CINO2	C20H18CINO2	C20H18CINO2
2-Chloro-4-[3-(4-chloro-phenoxy)- benzylamino]-phenol	4-[3-(4-tert-Butyl-phenoxy)- benzylamino]-2-chloro-phenol	4-(3-Benzyloxy-benzylamino)-2-chloro-phenol	4-(2-Benzyloxy-benzylamino)-2- chloro-phenol
		TI OF	TZ OF
1187	1188	1189	1190

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284.0	280.2	294.3	319.1	382.6
283.75	279.79	293.81	318.80	382.33
D	D	Д	D	Q
C17H14CINO	C14H14CINOS	C15H16CINOS	C17H19CIN2O2	C17H13Cl2NOS2
2-Chloro-4-[(naphthalen-1- ylmethyl)-amino]-phenol	2-Chloro-4-(4-methylsulfanyl- benzylamino)-phenol	2-Chloro-4-(2-ethylsulfanyl- benzylamino)-phenol	2-Chloro-4-(2-morpholin-4-yl-benzylamino)-phenol	2-Chloro-4-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol
IN SO	STEW STEW STEW STEW STEW STEW STEW STEW	D T		CO H
1191	1192	1193	1194	1195

					-	
1196	N HZ OH	2-Chloro-4-[(5-phenyl-2H-imidazol-4-ylmethyl)-amino]-phenol	C16H14CIN3O	Q	299.75	300.2
1197	TN D TO	4-[(5-Bromo-thiophen-2- ylmethyl)-amino]-2-chloro-phenol	C11H9BrCINOS	D	318.62	319.5
1198	20 HZ	2-Chloro-4-[3-(4-methoxy-phenol-phenol)	C20H18CINO3	Q	355.81	356.5
1199		2-Chloro-4-(3-methyl-benzylamino)-phenol	C14H14CINO	Q	247.72	248.5

	Structure	Chemical name	Formula	Synthesis methods	MolWeight	MS data
1200	HO CI-	2-Chloro-4-(3-trifluoromethyl- benzylamino)-phenol	C14H11CIF3NO	Q	301.69	302.2
1201	D D D	2-Chloro-4-(2-chloro-6-fluoro- benzylamino)-phenol	C13H10Cl2FNO	Q	286.13	286.6
1202	TZ OT	2-Fluoro-4-(3-phenoxy- benzylamino)-phenol	C19H16FNO2	Q	309.33	309.8
1203	TZ,	2-Fluoro-4-[3-(4-chloro-phenoxy)- benzylamino]-phenol	C19H15CIFNO2	Q	343.77	344.0

366.0	323.8	323.8	267.7	263.5
365.44	323.36	323.36	267.30	263.33
D	D	. О	D	A
C23H24FNO2	C20H18FNO2	C20H18FNO2	C17H14FNO	C14H14FNOS
4-[3-(4-tert-Butyl-phenoxy)- benzylamino]-2-fluoro-phenol	4-(3-Benzyloxy-benzylamino)-2- fluoro-phenol	4-(2-Benzyloxy-benzylamino)-2- fluoro-phenol	2-Fiuoro-4-[(naphthalen-1- ylmethyl)-amino]-phenol	2-Fluoro-4-(4-methylsulfanyl- benzylamino)-phenol
TZ Q	TZ Q			S TN DH
1204	1205	1206	1207	1208

277.8	302.8	366.0	283.8	302.5
277.36	302.34	365.87	283.30	302.16
Q	D	. О	Q	Q
C15H16FNOS	C17H19FN2O2	C17H13CIFNOS2	C16H14FN3O	C11H9BrFNOS
2-Fluoro-4-(2-ethylsulfanyl- benzylamino)-phenol	2-Fluoro-4-(2-morpholin-4-yl- benzylamino)-phenol	2-Fluoro-4-{[2-(4-chloro-phenylsulfanyl)-thiophen-3-ylmethyl]-amino}-phenol	2-Fluoro-4-[(5-phenyl-2H- imidazol-4-ylmethyl)-amino]- phenol	4-[(5-Bromo-thiophen-2- ylmethyl)-amino]-2-fluoro-phenol
TN OH	TZ,	HN NH	HO H	
1209	1210	1211	1212	1213

1214		2-Fluoro-4-[3-(4-methoxy-phenoy)-benzylamino]-phenol	C20H18FNO3	Q	339.36	339.8
1215	TZ Q	2-Fluoro-4-(3-methyl- benzylamino)-phenol	C14H14FNO	D	231.27	231.4
. 1216	HO CF.3	2-Fluoro-4-(3-trifluoromethyl- benzylamino)-phenol	C14H11F4NO	р .	285.24	285.5
1217	TZ TZ	2-Fluoro-4-(2-chloro-6-fluoro- benzylamino)-phenol	C13H10CIF2NO	D	269.67	270.1
1218	TN OH	2,6-Difluoro-4-(3-phenoxy- benzylamino)-phenol	C19H15F2NO2	Ω	327.32	327.6

362.0	383.8	341.7	341.7
361.76	383.43	341.35	341.35
D	Δ	D	Д
C19H14CIF2NO2	C23H23F2NO2	4-(3-Benzyloxy-benzylamino)-2,6-difluoro-phenol	C20H17F2NO2
2,6-Difluoro-4-[3-(4-chloro- phenoxy)-benzylamino]-phenol	2,6-Difluoro-4-[3-(4-chloro-phenoxy)-benzylamino]-phenol 4-[3-(4-tert-Butyl-phenoxy)-benzylamino]-2,6-difluoro-phenol		4-(2-Benzyloxy-benzylamino)-2,6- difluoro-phenol
TZ U	TZ u	TZ, u,	IZ U
1219	1220	1221	1222

285.6	281.6	295.7	320.8	384.2
285.29	281.32	295.35	320.33	383.86
Q	Д	Q	Q	Д
C17H13F2NO	C14H13F2NOS	C15H15F2NOS	C17H18F2N2O2	C17H12CIF2NOS2
2,6-Difluoro-4-[(naphthalen-1- ylmethyl)-amino]-phenol	2,6-Difluoro-4-(4-methylsulfanyl- benzylamino)-phenol	2,6-Difluoro-4-(2-ethylsulfanyl- benzylamino)-phenol	2,6-Difluoro-4-(2-morpholin-4-yl- benzylamino)-phenol	2,6-Difluoro-4-{[2-(4-chloro-phenylsulfanyl}-thiophen-3-ylmethyl]-amino}-phenol
TZ u.	STN DH	TZ U	TZ UL	HO S S
1223	1224	1225	1226	1227

1228	IZ U OH	2,6-Difluoro-4-[(5-phenyl-2H- imidazol-4-ylmethyl)-amino]- phenol	C16H13F2N3O	Q	301.29	301.6
1229	m of m	4-[(5-Bromo-thiophen-2- ylmethyl)-amino]-2,6-difluoro- phenol	C11H8BrFZNOS	Q	320.15	320.4
1230	TZ O	2,6-Difluoro-4-[3-(4-methoxy- phenoxy)-benzylamino]-phenol	C20H17F2NO3	D	357.35	357.6
1231	TN OF	2,6-Difluoro-4-(3-methyl- benzylamino)-phenol	C14H13FZNO	Q ·	249.26	249.6
1232	TX QT	2,6-Difluoro-4-(3-trifluoromethyl- benzylamino)-phenol	C14H10F5NO	О	303.23	303.7

288.1	279.8	245.6	301.8	. 231.7
287.66	279.31	245.30	301.40	231.27
Q	В	М	<b>.</b>	Д
C13H9CIF3NO	C13H13NO4S	C10H15NO4S	C14H23NO4S	C9H13NO4S
2,6-Difluoro-4-(2-chloro-6-fluoro- benzylamino)-phenol	N-(2,4-Dihydroxy-phenyl)-C- phenyl-methanesulfonamide	Butane-1-sulfonic acid (2,4-dihydroxy-phenyl)-amide	Octane-1-sulfonic acid (2,4- dihydroxy-phenyl)-amide	Propane-2-sulfonic acid (2,4-dihydroxy-phenyl)-amide
IZ OF	HN-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-	HN OHO	N HO OH	OHN——OH
1233	1234	1235	1236	1237

332.4	298.5	354.6	284.5	297.9
332.20	298.19	354.29 <sub>(</sub>	284.16	297.76
<b>M</b>	В	В	В	В
C13H11CIZNO3S	C10H13CI2NO3S	C14H21CI2NO3S	C9H11CI2NO3S	C13H12CINO3S
N-(3,5-Dichloro-4-hydroxy-phenyl)-C-phenyl-methanesulfonamide	Butane-1-sulfonic acid (3,5-dichloro-4-hydroxy-phenyl)-amide	Octane-1-sulfonic acid (3,5-dichloro-4-hydroxy-phenyl)-amide	Propane-2-sulfonic acid (3,5-dichloro-4-hydroxy-phenyl)-amide	N-(3-Chloro-4-bydroxy-phenyl)- C-phenyl-methanesulfonamide
HONON	HO CO	JZ OJ	HOOH	HO NH O
1238	1239	1240	1241	1242

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1243	HOHOM	Butane-1-sulfonic acid (3-chloro-4-hydroxy-phenyl)-amide	C10H14CINO3S	В	263.74	264.0
1244	HONT	Octane-1-sulfonic acid (3-chloro-4-hydroxy-phenyl)-amide	C14H22CINO3S	α.	319.85	320.3
1245	HO	Propane-2-sulfonic acid (3-chloro-4-hydroxy-phenyl)-amide	C9H12CINO3S	В	249.71	250.4
	HO NH O	N-(3-Fluoro-4-hydroxy-phenyl)-C-phenyl-methanesulfonamide	C13H12FNO3S	В	281.30	281.8
1247	HOHON	Butane-1-sulfonic acid (3-fluoro-4-hydroxy-phenyl)-amide	C10H14FNO3S	В	247.29	. 247.8

3.8	233.7	300.8	265.7	321.8
303.8	23.	30	56	
303.39	233.26	299.29	265.28	321.38
Ф	Д	щ	<b>.</b>	В
C14H22FNO3S	C9H12FNO3S	C13H11F2NO3S	C10Hi3F2NO3S	C14H21F2NO3S
Octane-1-sulfonic acid (3-fluoro-4-   C	Propane-2-sulfonic acid (3-fluoro- 4-hydroxy-phenyl)-amide	N-(3,5-Difluoro-4-hydroxy- phenyl)-C-phenyl- methanesulfonamide	Butane-1-sulfonic acid (3,5- cifluoro-4-hydroxy-phenyl)-amide	Octane-1-sulfonic acid (3,5- (difluoro-4-hydroxy-phenyl)-amide
IN DE	HO	HOHON	HOH	O D O T
1248	1249	1250	1251	1252

251.6	253.7	306.4	272.1	255.6
251.25	253.29	306.18	271.74	255.29
В	F, G, H	F, G, H	F, G, H	F, G, H
C9H11F2NO3S	C13H19NO4	C13H17Cl2NO3	C13H18CINO3	C13H18FNO3
Propane-2-sulfonic acid (3,5-difluoro-4-hydroxy-phenyl)-amide	(2,4-Dihydroxy-phenyl)-carbamic acid hexyl ester	(3,5-Dichloro-4-hydroxy-phenyl)- carbamic acid hexyl ester	(3-Chloro-4-hydroxy-phenyl)- carbamic acid hexyl ester	(3-Fluoro-4-hydroxy-phenyl)- carbamic acid hexyl ester
HN HN H	F OF OF OF OF	HO IN THE REPORT OF THE PERSON	F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	F
1253	1254	1255	1256	1257

1258	F	(3,5-Dibromo-4-hydroxy-phenyl)- carbamic acid hexyl ester	C13H17Br2NO3	F, G, H	395.09	395.3
1259	# T T T T T T T T T T T T T T T T T T T	(3,5-Diftuoro-4-hydroxy-phenyl)- carbamic acid hexyl ester	C13H17F2NO3	F, G, H	273.28	273.6
1260	TZ O	-[3-(2,4-Dihydroxy-phenyl)- ureido]-4-methyl-pentanoic acid ethyl ester	acid C15H22N2O5	·	310.35	310.7
1261	TZ O TZ O T	2-[3-(3,5-Dichloro-4-hydroxy-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	C15H20Cl2N2O4	∢	363.24	363.6
1262	TZ O	2-[3-(3-Chloro-4-hydroxy-phenyl)- ureido]-4-methyl-pentanoic acid ethyl ester	C15H21CIN2O4	¥	328.79	329.1

312.8	330.8	452.3	344.8	397.6
312.34	330.33	452.14	344.36	397.25
A	Ą	V	Ą	Ą
C15H21FN2O4	C15H20F2N2O4	C15H20Br2N2O4	C18HZ0NZOS	C18H18Cl2N2O4
2-[3-(3-Fluoro-4-hydroxy-phenyl)- ureido]-4-methyl-pentanoic acid ethyl ester	2-[3-(3,5-Difluoro-4-hydroxy-4-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	2-[3-(3,5-Dibromo-4-hydroxy-4-methyl-phenyl)-ureido]-4-methyl-pentanoic acid ethyl ester	2-[3-(2,4-Dihydroxy-phenyl)- ureido]-3-phenyl-propionic acid ethyl ester	2-[3-(3,5-Dichloro-4-hydroxy-phenyl)-ureido]-3-phenyl-propionic acid ethyl ester
TZ O TZ	TZ O LL	HZ O H	IZ O	TZ O
1263	1264	1265	1266	1267

363.0	346.7	364.8	486.2
362.81	346.35	364.34	486.15
¥	∢	¥	¥
C18H19CIN2O4	C18H19FN2O4	C18H18F2N2O4	C18H18Br2N2O4
2-[3-(3-Chloro-4-hydroxy-phenyl)- ureido]-3-phenyl-propionic acid ethyi ester	2-[3-(3-Fluoro-4-hydroxy-phenyl)- ureido]-3-phenyl-propionic acid ethyl ester	2-[3-(3,5-Difluoro-4-hydroxy- phenyl)-ureido]-3-phenyl- propionic acid ethyl ester	2-[3-(3,5-Dibromo-3-fluoro-4- hydroxy-phenyl)-ureido]-3-phenyl- propionic acid ethyl ester
TZ O	TZ O	IZ O	IN OH
1268	1269	1270	1271

	-			
265.7	318.5	284.0	267.7	285.7
265.35	318.24	283.79	267.34	285.33
ບ	ນ	O	ပ	S
C15HZ3NO3	CISHZICIZNOZ	C15H22CINO2	C15H21FNO2	C15H21F2NO2
3,5,5-Trimethyl-hexanoic acid (2,4-dihydroxy-phenyl)-amide	3,5,5-Trimethyl-hexanoic acid (3,5-dichloro-4-hydroxy-phenyl)- amide	3,5,5-Trimethyl-hexanoic acid (3- chloro-4-hydroxy-phenyl)-amide	3,5,5-Trimethyl-hexanoic acid (3-fluoro-4-hydroxy-phenyl)-amide	3,5,5-Trimethyl-hexanoic acid (3,5-difluoro-4-hydroxy-phenyl)- amide
HO HO	D OF	TZ 5 g	TZ OF	TZ u
1272	1273	1274	1275	1276

407.3	376.1	410.1	424.1
407.14	375.9	409.9	423.9
ນ	K followed by A	K followed by A	K followed by A
C15H21Br2NO2	C18H18CIN3O2S	C21H16CIN3O2S	C22H18CIN3O2S
3,5,5-Trimethyl-hexanoic acid (3,5-dibromo-4-hydroxy-phenyl)-amide	1-(3-Benzothiazol-2-yl-5-chloro-4- hydroxy-phenyl)-3-tert-butyl-urea	1-(3-Benzothiazol-2-yl-5-chloro-4- hydroxy-phenyl)-3-benzyl-urea	1-(3-Benzothiazol-2-yl-5-chloro-4- hydroxy-phenyl)-3-phenethyl-urea
HN Page 1	S IZ O	S IZ O	S IN S
1277	1278	1279	1280

378.1	392.1	417.2
377.9	391.9	417.0
K followed by	K followed by I	K followed by C
C17H16CIN3OS2	C18H18CIN3OS2	C22H25CIN2O2S
1-(3-Benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-3-isopropyl-thiourea	1-(3-Benzothiazol-2-yl-5-chloro-4- hydroxy-phenyl)-3-tert-butyl- thiourea	3,5,5-Trimethyl-hexanoic acid (3-benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-amide
HO NH NH S	D IN	5 S
1281	1282	1283

	\(\frac{1}{2}\)		•			
S	NH NH	N-(3-Benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-3-phenyl-propionamide	C22H17CIN2O2S	K followed by C	408.9	409.2
Ę	IZ D	1-(4-Hydroxy-2-methyl-phenyl)-3- C13H20N2O2 pentyl-urea	C13H20N2O2	Ą	263.31	256.9
오	HO N	Biphenyl-4-carboxylic acid (2,4- dihydroxy-phenyl)-amide	C19H15NO3	. 選つ	305.33	305.6
· · · · · · · · · · · · · · · · · · ·	TZ 5	Biphenyl-4-carboxylic acid (3,5- dichloro-4-hydroxy-phenyl)-amide	CZ0H15ClZNO2	C, E	358.22	358.5
	H- H	4-[(Furan-2-ylmethyl)-amino]- benzene-1,3-diol	C11H11NO3	D	205.21	205.7

258.4	225.7	283.5	303.6	310.4
258.10	225.19	283.25	303.23	310.18
D	Q	· Q	Œ	C, E
C11H9Cl2NO2	C11H9F2NO2	C14H12F3NO2	C14H10F5NO	C15H13Cl2NO2
2,6-Dichloro-4-[(furan-2- ylmethyl)-amino]-phenol	2,6-Difluoro-4-[(furan-2- ylmethyl)-amino]-phenol	4-(2-Trifluoromethyl- benzylamino)-benzene-1,3-diol	2,6-Difluoro-4-(2-trifluoromethyl- benzylamino)-phenol	N-(3,5-Dichloro-4-hydroxy- phenyl)-3-phenyl-propionamide
D P	TZ Q	HO OH	HN HO	HO TO
1289	1290	1291	1292	1293

341.3	340.3	260.2	332.4	282.3
341.15	340.16	260.12	332.18	282.12
C, B	C, B	ີ .	C, B	C, E
C14H10CI2N2O4	C15H11CIZNO4	C11H11Cl2NO2	C17H11CI2NO2	C13H9Cl2NO2
N-(3,5-Dichloro-4-hydroxy- phenyl)-2-(2-nitro-phenyl)- acetamide	2-Benzo[1,3]dioxol-5-yl-N-(3,5-dichloro-4-hydroxy-phenyl)-acetamide	3-Methyl-but-2-enoic acid (3,5- dichloro-4-hydroxy-phenyl)-amide	Naphthalene-2-carboxylic acid (3,5-dichloro-4-hydroxy-phenyl)- amide	N-(3,5-Dichloro-4-hydroxy- phenyl)-benzamide
D OH OH	O TO	D TZ D D	DO TEX	TZ 5
1294	1295	1296	1297	1298

272.3	336.5
272.08	336.14
C, B	Ω
C11H7CI2NO3	C14H10Cl2F3NO
Furan-2-carboxylic acid (3,5- dichloro-4-hydroxy-phenyl)-amide	2,6-Dichloro-4-(2-trifluoromethyl- benzylamino)-phenol
CI HO	CI N CF3
1299	1300

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or a pharmaceutical acceptable salt or prodrug thereof.

Even more preferred compounds according to the present invention are those mentioned in any of the tables herein and those further disclosed and/or characterized in the examples.

As used herein, each of the following terms, used alone or in conjunction with other terms, are preferably used in the following meaning (except where noted to the contrary):

The term "alkyl" refers to a saturated aliphatic radical containing from one to ten carbon atoms or a mono- or polyunsaturated aliphatic hydrocarbon radical containing from two to twelve carbon atoms, containing at least one double and triple bound, respectively. "Alkyl" refers to both branched and unbranched alkyl groups. Preferred alkyl groups are straight chain alkyl groups containing from one to eight carbon atoms. More preferred alkyl groups are straight chain alkyl groups containing from one to six carbon atoms and branched alkyl groups containing from three to six carbon atoms. It should be understood that any combination term using an "alk" or "alkyl" prefix refers to analogs according to the above definition of "alkyl". For example, terms such as "alkoxy", "alkylthio" refer to alkyl group linked to a second group via an oxygen or sulfur atom. "Alkanoyl" refers to an alkyl group linked to a carbonyl group (C=O). "Substituted alkyl" refers to alkyl groups straight or branched further bearing one or more substituents. One substituent also means monosubstituted and more substitutents mean poly-substituted. It should be understood that any combination term using a "substituted alkyl" prefix refers to analogs according to the above definition of "substituted alkyl". For example, a term such as "substituted alkylaryl" refers to substituted alkyl group linked to an aryl group.

The term "cycloalkyl" refers to the cyclic analog of an alkyl group, as defined above, optionally unsaturated and/or substituted. Preferred cycloalkyl groups are saturated cycloalkyl groups, more particularly those containing from three to eight carbon atoms, and even more preferably three to six carbon atoms. "Substituted cycloalkyl" refers to cycloalkyl groups further bearing one or more substituents. "Mono-unsaturated cycloalkyl" refers to cycloalkyl containing one double bond or one triple bond. "Poly-unsaturated cycloalkyl" refers to cycloalkyl containing at least two double bonds or two triple bonds or a combination of at least one double bond and one triple bond.

The term "alkenyl" refers to an unsaturated hydrocarbon group containing at least one carbon-carbon double bond, including straight-chain, branched-chain, and cyclic groups. Preferred alkenyl groups have one to twelve carbons. More preferred alkenyl groups have one to six carbons. "Substituted alkenyl" refers to alkenyl groups further bearing one or more substitutents.

The term "cycloalkenyl" refers to the cyclic analog of an alkenyl group, as defined above, optionally substituted. Preferred cycloalkenyl groups are containing from four to eight carbon atoms. "Substituted cycloalkenyl" refers to cycloalkenyl groups further bearing one or more substituents. "Mono-unsaturated cycloalkenyl" refers to cycloalkenyl containing one double bond. "Poly-unsaturated cycloalkenyl" refers to cycloalkenyl containing at least two double bonds.

The term "alkynyl" refers to an unsaturated hydrocarbon group containing at least one carbon-carbon triple bond, including straight-chain, branched-chain, and cyclic groups. Preferred alkynyl groups have one to twelve carbons. More preferred alkynyl groups have one to six carbons. "Substituted alkynyl" refers to alkynyl groups further bearing one or more substitutents.

The term "aryl" refers to aromatic groups having in the range of 6 to 14 carbon atoms and "substituted aryl" refers to aryl groups further bearing one or more substituents. It should be understood that any combination term using an "ar" or "aryl" prefix refers to analogs according to the above definition of "aryl". For example, a term such as "aryloxy" refers to aryl group linked to a second group via an oxygen.

Each of the above defined "alkyl", "cycloalkyl", and "aryl" shall be understood to include their halogenated analogs, whereby the halogenated analogs may comprise one or several halogen atoms. The halogenated analogs thus comprise any halogen radical as defined in the following.

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The term "halo" refers to a halogen radical selected from fluoro, chloro, bromo, iodo. Preferred halo groups are fluoro, chloro and bromo.

The term "heteroaryl" refers to a stable 5 to 8 membered, preferably 5 or 6 membered monocyclic or 8 to 11 membered bicyclic aromatic heterocycle radical. Each heterocycle consists of carbon atoms and from 1 to 4 heteroatoms selected from the group consisting of nitrogen, oxygen, sulfur. The heterocycle may be attached by any atom of the cycle, which preferably results in the creation of a stable structure. Preferred heteroaryl radicals as used herein include, for example, furanyl, thienyl, pyrrolyl, oxazolyl, thiazolyl, imidazolyl, pyrazolyl, isoxazolyl, isothiazolyl, oxadiazolyl, triazolyl, tetrazolyl, thiadiazolyl, pyridinyl, pyridazinyl, pyrimidinyl, pyrazinyl, indolizinyl, indolyl, isoindolyl, benzofuranyl, benzothienyl, indazolyl, benzimidazolyl, benzthiazolyl, benzoxazolyl, purinyl, quinolizinyl, quinolinyl, isoquinolinyl, cinnolinyl, phthalazinyl, quinazolinyl, quinoxalinyl, naphthridinyl, pteridinyl, carbazolyl, acridinyl, phenazinyl, phenothiazinyl and phenoxazinyl. "Substituted heteroaryl" refers to heteroaryl groups further bearing one or more substituents.

The term "heterocyclyl" refers to a stable 5 to 8 membered, preferably 5 or 6 membered monocyclic or 8 to 11 membered bicyclic heterocycle radical which may be either saturated or unsaturated, and is non-aromatic. Each heterocycle consists of carbon atom(s) and from 1 to 4 heteroatoms selected from the group consisting of nitrogen, oxygen and sulfur. The heterocycle may be attached by any atom of the cycle, which preferably results in the creation of a stable structure. Preferred heterocycle radicals as used herein include, for example, pyrrolinyl, pyrrolidinyl, pyrazolinyl, pyrazolidinyl, piperidinyl, morpholinyl, thiomorpholinyl, tetrahydropyranyl, indolinyl, azetidinyl, piperazinyl, pyranyl, thiopyranyl, tetrahydrothiopyranyl, tetrahydrofuranyl, hexahydropyrimidinyl, hexahydropyridazinyl, 1,4,5,6-tetrahydropyrimidin-2-ylamine, dihydro-oxazolyl, 1,2-thiazinanyl-1,1-dioxide, 1,2,6thiadiazinanyl-1,1-dioxide, isothiazolidinyl-1,1-dioxide and imidazolidinyl-2,4-dione. "Mono-unsaturated heterocyclyl" refers to heterocyclyl containing one double bond or one triple bond. "Poly-unsaturated heterocyclyl" refers to heterocyclyl containing at least two double bonds or two triple bonds or a combination of at least one double bond and one triple bond.

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"Substituted heterocyclyl" refers to heterocyclyl groups further bearing one or more substituents.

The terms "heterocyclyl", "heteroaryl" and "aryl", when associated with another moiety, unless otherwise specified, shall have the same meaning as given above. For example, "aroyl" refers to phenyl or naphthyl linked to a carbonyl group (C=O).

Each aryl or heteroaryl unless otherwise specified includes its partially or fully hydrogenated derivative. For example, quinolinyl may include decahydroquinolinyl and tetrahydroquinolinyl, naphthyl may include its hydrogenated derivatives such as tetrahydranaphthyl.

As used herein above and throughout this application, "nitrogen" or "N'and "sulfur" or "S" include any oxidized form of nitrogen and sulfur and the quaternized form of any basic nitrogen sulfoxide, sulfone, nitrone, N-oxide.

As used herein a wording defining the limits of a range of length such as e. g. "from 1 to 5" means any integer from 1 to 5, i. e. 1, 2, 3, 4 and 5. In other words, any range defined by two integers explicitly mentioned is meant to comprise any integer defining said limits and any integer comprised in said range.

As used herein the term substituted shall mean that one or more H atom of the group or compound which is substituted, is replaced by a different atom, a group of atoms, a molecule or a molecule moiety. Such atom, group of atoms, molecule or molecule moiety is also referred to herein as substituent.

The substituent can be selected from the group comprising hydroxy, alkoxy, mercapto, cycloalkyl, heterocyclic, aryl, heteroaryl, aryloxy, halogen, trifluoromethyl, difluoromethyl, cyano, nitrone, amino, amido, -C(O)H, acyl, oxyacyl, carboxyl, carbamate, sulfonyl, sulphonamide and sulfuryl. Any of the substituents may be substituted itself by any of the aforementioned substituents. This applies preferably to cycloalkyl, heterocylic, aryl, heteroaryl and aryloxy. It is also preferred that alkoxy and mercapto are those of a lower alkyl

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group. It is to be acknowledged that any of the definition provided herein also applies to any substituent.

A substituent can also be any of R<sup>a</sup>, R<sup>b</sup>, R<sup>c</sup>, R<sup>d</sup>, R<sup>e</sup>, R<sup>f</sup>, and R<sup>g</sup> and/or any of R<sub>1</sub> to R<sub>21</sub>. It is also within the present invention that any substitutent may in turn be substituted by a substituent. A group, structure, moiety or the like which is substituted may comprise several substituents which may either be different or the same.

As used herein =T can mean in any embodiment of the various aspects of the present invention that with =T is selected from electron withdrawing groups, whereby preferably the electron withdrawing groups are selected from =O, =N-R<sup>e</sup>, =N-CN, =N-NO<sub>2</sub> and =CH-NO<sub>2</sub>, and =S,

It is within the present invention that any thiourea moieties and derivates therefrom, particularly those described herein, can, in principle be replaced by a cyanoguanidine moiety or residue and respective derivates therefrom as described in J. Med. Chem 1977, 20, 901 – 906. In Addition to being weakly basic cyanoguanidine and thiourea are also weakly acidic and both are therefore neutral and weakly amphoteric compounds. Cyanoguanidine is also similar to thiourea in its geometry since both are planar structures with almost identical C-N bond lengths and bond angles. Another property common to thioureas and cyanoguanidines is conformational isomerism resulting from restricted C-N bond rotation. Cyanoguanidine and thiourea are similar in their hydrophilicity and hydrogen-bonding properties; they have comparably low octanol-water partition coefficients (P) and are both reasonably soluble in water.

As used herein in connection with an embodiment of the various aspects of the present invention the term "wherein R<sub>1</sub> and R<sub>2</sub>, R<sub>2</sub> and R<sub>3</sub>, R<sub>3</sub> and R<sub>4</sub>, R<sub>1</sub> and R<sub>3</sub>, R<sub>1</sub> and R<sub>4</sub>, or R<sub>2</sub> and R<sub>4</sub> may be linked so as to form a ring comprising 4 to 12 members, preferably 5 to 10 members" shall mean that any of the two residues R, such as, for example, R<sub>1</sub> and R<sub>2</sub> or R<sub>2</sub> and R<sub>3</sub>, are linked to each through a covalent bond, a non-covalent bond or any combination thereof. The formation of the ring may be the result of one or several of this kind of bonds. It is to be understood that the molecule may comprise one or more of those rings formed by two residues R.

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In a preferred embodiment wherein R<sub>1</sub> and R<sub>2</sub>, R<sub>2</sub> and R<sub>3</sub>, R<sub>3</sub> and R<sub>4</sub>, R<sub>1</sub> and R<sub>3</sub>, R<sub>1</sub> and R<sub>4</sub>, or R<sub>2</sub> and R<sub>4</sub> linked so as to form a ring comprising 4 to 12 members, preferably 5 to 10 members, more preferably 5 or 6 members, R1, R2, R3 and R4 are each and independently selected from the group comprising H, OR6, SR7, NR8R9, halo, alkyl, substituted alkyl, alkylaryl, substituted alkylaryl, cycloalkyl, substituted cycloalkyl, alkylcycloalkyl, substituted heterocyclyl, substituted heterocyclyl, substituted aryl, alkylcycloalkyl, aryl, alkylheterocyclyl, heteroaryl, heteroaryl, substituted alkylheterocyclyl, substituted alkylheteroaryl and substituted alkylheteroaryl;

The ring may be cycloalkyl, heterocyclyl, aryl, or heteroaryl. The cycloalkyl or heterocyclyl ring can be mono-unsaturated or poly-unsaturated. The ring can be substituted by one or more substituents as defined herein

As used herein in connection with an embodiment of the various aspects of the present invention the term "each and independently selected from a group" or "are independently from each other selected from the group" refers to two or more atoms, groups, substituents, moieties or whatsoever and describes that the single atom, group etc. mentioned can be selected from the group. The wording used is a truncation which avoids unnecessary repetition as otherwise for each of the atoms, groups etc. the same group definition would have to be repeated.

As used herein in connection with an embodiment of the various aspects of the present invention the term "each and individually absent" refers to two or more atoms, groups, substituents, moieties or whatsoever and describes that the single atom, group etc. mentioned can be absent regardless whether any of the other atoms, groups etc. mentioned is absent. The wording used is a truncation which avoids unnecessary repetition as otherwise for each of the atoms, groups etc. the fact that it may be absent in an embodiment of the invention would have to be repeated.

In connection with the present invention some groups such as, e.g.,  $-(CR^aR^b)$ — or  $-(CR^fR^g)$ —are repeated, i.e. are repeatedly present in a compound according to the present invention. Typically such repetition occurs in such a manner that, e.g.,  $-(CR^aR^b)$ — is repeated one or

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several times. In case, e.g.,  $-(CR^aR^b)$ — is repeated one time which means that there are two consecutive groups of  $-(CR^aR^b)$ —, these two forms of  $-(CR^aR^b)$ — can be either the same or they may be different in a different embodiment which means that either  $R^a$  or  $R^b$  or both of them are different between said two  $-(CR^aR^b)$ — groups. If there are three or more of these groups such as , e.g.,  $-(CR^aR^b)$ —, it is possible that all of them are different or only some or different whereas others are the same in the sense defined above. Any permutation for the arrangement for such identical or different groups is within the present invention.

The same applies to the design and arrangement of the spacer -M1-L1-K-L2-M2-.

In connection with any of the compounds according to the present invention and more particularly in connection with the compounds according to formulae VI to XIII and XIX to XXVI it is to be noted that the formation of a ring structure through E between the cyclic moiety A such as the phenol moiety and the spacer X can occur between the cyclic moiety A such as the phenol moiety and any of the spacer moieties -M1-L1-K-L2-M2-, regardless whether they are of a linear or any of the cyclic structures themselves. It is therefore within the present invention that in case of a repetition of the above described spacer moiety -M1-L1-K-L2-M2- the ring formation can either occur at the -M1-L1-K-L2-M2- moiety which is next or closest to the ring as represented in the respective formulae, or at the or any of the further -M1-L1-K-L2-M2- moieties present in the particular compound.

As used herein in connection with an embodiment of the various aspects of the present invention the term C=T shall represent a C atom having a double bond with T which represents certain atoms, groups, substituents, moieties or the like as further defined herein.

It is within the present invention that the features of the various embodiments of the present invention can be realized either alone or in combination with the features of any other embodiment(s) of the present invention. Thus any combination of an/the individual feature or the combination of features of an embodiment of the present invention with an/the individual feature(s) or the combination of features of any other embodiment(s), either alone or in combination with other embodiments, shall be disclosed by the present specification.

As used herein in connection with an embodiment of the various aspects of the present invention the term referring to a group, substituent, moiety, spacer or the like specifying that it "can be inserted in any orientation into any of the preceding formulae" means that the group etc. can be attached to another atom, group, substitutent, moiety spacer or the like of any of the compounds according to the present invention or any of the formulae disclosed herein via any of its ends an in particular through any of the atoms arranged at the ends of said group, substituent, moiety, spacer or the like.

In a further aspect the present invention is related to the use of a compound according to any of the aspects of the present invention as an inhibitor to or for a rotamase.

In an embodiment the rotamase regulates a part of the cell cycle.

In a preferred embodiment the rotamase regulates a part of the cell cycle, whereby preferably the part of the cell cycle is mitosis.

In an even more preferred embodiment the rotamase is a mammalian rotamase, preferably a human rotamase, more preferably hPin1.

In a further aspect the present invention is related to the use of the compounds according to the present invention as a pharmaceutical or in a pharmaceutical composition or for the manufacture of such pharmaceutical composition which is preferably for the prophylaxis and/or treatment of a disease, whereby the disease involves a rotamase, whereby the rotamase is a mammalian rotamase, preferably a human rotamase, more preferably hPin1.

In connection with the further aspect of the present invention related to the use of any of the aforementioned compounds according to the present invention as an inhibitor to rotamases the following will be acknowledged by the one skilled in the art. In view of the characteristics of the compounds according to the present invention to be active as an inhibitor of (a) rotamase(s), it is sufficient that the respective compound is at least suitable to inhibit at least one rotamase. The compounds according to the present invention which may be used as inhibitors, are also referred to as rotamase inhibitors herein.

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Rotamases as such are known in the art and, for example, described in the introductory part of this specification which is incorporated by reference. Rotamases as used herein shall mean cyclophilins, FK-506 binding proteins and the rotamases of the Pin1/parvulin class. The Pin1/parvulin class includes Pins 1 to 3, PinL/parvulin, dodo, and Es1/Pft1. Suitable assays to determine whether a compound is suitable to inhibit a rotamase are known to the one skilled in the art and also described in the present examples. Basically, a rotamase is provided the activity of which or non-activity of which may be determined. A candidate inhibitor, i. e. a compound which is to be tested whether it is active as an inhibitor to rotamase, is added to the rotamase and tested whether upon the addition and/or influence of the candidate inhibitor the activity of the rotamase is changed relative to the activity without candidate rotamase inhibitor. If the rotamase activity is decreased by the candidate rotamase inhibitor, said candidate rotamase inhibitor is a rotamase inhibitor according to the present invention.

In another aspect of the present invention the compounds according to the present invention may be used in a method for inhibiting a rotamase. In such case a rotamase is provided and a candidate rotamase inhibitor is added thereto whereupon the activity of rotamase is decreased. Optionally, such decrease in rotamase activity is measured. The techniques used theretofore are basically the same as outlined in connection with the use of the compounds according to the present invention as rotamase inhibitors.

The compounds according to the present invention are preferably reversible rotamase inhibitors.

By "reversible" herein is meant that the inhibitor binds non-covalently to the enzyme, and is to be distinguished from irreversible inhibition. See Walsh, Enzymatic Reaction Mechanisms, Freeman & Co., N.Y., 1979. "Reversible" in this context is a term understood by those skilled in the art. Preferably the rotamase inhibitors according to the present invention are competitive inhibitors, that is, they compete with substrate in binding reversibly to the enzyme, with the binding of inhibitor and substrate being mutually exclusive.

In a preferred embodiment of the compounds according to the present invention being active as a rotamase inhibitor, the dissociation constant for inhibition of a rotamase with the inhibitor, generally referred to and characterized by those in the art as  $K_i$ , is at most about 100

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μM. By the term "binding constant" or "dissociation constant" or grammatical equivalents herein is meant the equilibrium dissociation constant for the reversible association of inhibitor with enzyme. The dissociation constants are defined and determined as described below. The determination of dissociation constants is known in the art. For example, for reversible inhibition reactions such as those of the present invention, the reaction scheme is as follows:

E+I 
$$\frac{k_1}{k_2}$$
 E\*I (Equation 1)

The enzyme (E) and the inhibitor (I) combine to give an enzyme-inhibitor complex (E\*I). This step is assumed to be rapid and reversible, with no chemical changes taking place; the enzyme and the inhibitor are held together by non-covalent forces. In this reaction,  $k_1$  is the second order rate constant for the formation of the E\*I reversible complex.  $k_2$  is the first order rate constant for the dissociation of the reversible E\*I complex. In this reaction,  $K_1 = k_2/k_1$ .

The measurement of the equilibrium constant  $K_i$  proceeds according to techniques well known in the art, as described in the examples. For example, assays generally use synthetic chromogenic or fluorogenic substrates. The respective  $K_i$  values may be estimated using the Dixon plot as described by Irwin Segel in Enzyme Kinetics: Behavior and analysis of rapid equilibrium and steady-state enzyme systems, 1975, Wiley-Interscience Publication, John Wiley & Sons, New York, or for competitive binding inhibitors from the following calculation:

$$1-(v_i/v_o)=[I]/[I]+K_i (1+([S]/K_m)))$$
 (Equation 2)

wherein  $v_0$  is the rate of substrate hydrolysis in the absence of inhibitor, and  $v_i$  is the rate in the presence of competitive inhibitor.

It is to be understood that dissociation constants are a particularly useful way of quantifying the efficiency of an enzyme with a particular substrate or inhibitor, and are frequently used in the art as such. If an inhibitor exhibits a very low  $K_i$  value, it is an efficient inhibitor. Accordingly, the rotamase inhibitors of the present invention have dissociation constants,  $K_i$ ,

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of at most about 100  $\mu$ M. Preferably, the rotamase inhibitors according to the present invention exhibit dissociation constants of at most about 10  $\mu$ M, more preferably about 1  $\mu$ M, most preferably of at most about 100 nM.

The rotamase inhibitors of the present invention may be easily screened for their inhibitory effect. The inhibitor is first tested against different classes of rotamases for which the targeting group of the inhibitor was chosen, as outlined above. The activity of rotamases is typically measured by using a protease coupled assay with chromogenic substrates and conformer specific proteases. Basically, upon the conformer specific protease activity the chromogenic substrate is converted into a compound which has an absorption characteristic which is different from the starting chromogenic substrate and may thus be selectively measured. This reaction is accelerated in presence of the rotamase and decelerated in the presence of rotamase-inhibitors. Alternatively, many rotamases and their corresponding chromogenic substrates are commercially available. Thus, a variety of rotamases are routinely assayed with synthetic chromogenic substrates in the presence and absence of the rotamase inhibitor, to confirm the inhibitory action of the compound, using techniques well known in the art. The effective inhibitors are then subjected to kinetic analysis to calculate the K<sub>i</sub> values, and the dissociation constants determined.

If a compound inhibits at least one rotamase, it is a rotamase inhibitor for the purposes of the present invention. Preferred embodiments of the rotamase inhibitors according to the present invention are compounds and inhibitors, respectively, that exhibit the correct kinetic parameters Ki below 100  $\mu$ M against the targeted rotamases.

In a further aspect of the present invention any of the compounds used as rotamase inhibitors or as a medicament may be labelled.

By a "labelled rotamase inhibitor" herein is meant a rotamase inhibitor that has at least one element, isotope or chemical compound attached to enable the detection of the rotamase inhibitor or the rotamase inhibitor bound to a rotamase. In general, labels as used herein, fall into three classes: a) isotopic labels, which may be radioactive or heavy isotopes; b) immune labels, which may be antibodies or antigens; and c) colored or fluorescent dyes. The labels

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may be incorporated into the rotamase inhibitor at any position. Examples of useful labels include <sup>14</sup>C, <sup>13</sup>C, <sup>15</sup>N, <sup>3</sup>H, biotin, and fluorescent labels as are well known in the art.

In a further aspect the compounds according to the present invention, particularly those having rotamase inhibitory activity, may be used for removing, identifying and/or inhibiting contaminating rotamases in a sample.

Therefore, the rotamase inhibitors of the present invention are, for example, added to a sample where the catalytic activity by contaminating rotamases is undesirable. Alternatively, the rotamase inhibitors of the present invention may be bound to a chromatographic support, using techniques well known in the art, to form an affinity chromatography column. A sample containing an undesirable rotamase is run through the column to remove the rotamase. Alternatively, the same methods may be used to identify new rotamases. In doing so, a new rotamase contained in a sample may bind to the rotamase inhibitor bound to the chromatographic support and upon elution, preferably a specific elution, from said chromatographic support, characterized and compared to other rotamase activities with regard to, among others, specificities. The characterization of the rotamase as such is known to the one skilled in the art.

In a further aspect the present invention is related to a pharmaceutical composition comprising a compound according to any of the aspects of the present invention and a pharmaceutically acceptable carrier, diluent or excipient.

In an embodiment the composition comprises a further pharmaceutically active compound, preferably such further pharmaceutically active compound is a chemotherapeutic agent.

In a preferred embodiment of the composition the compound is present as a pharmaceutically acceptable salt or a pharmaceutically active solvate.

In an even more preferred embodiment the pharmaceutically active compound is either alone or in combination with any of the ingredients of the composition present in a multitude of individualized dosages and/or administration forms.

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The use of the compounds according to the present invention for the manufacture of a medicament is based on the fact that the compounds according to the present invention are inhibitors of rotamases and rotamases in turn have been identified in both procaryotic and eucaryotic cells such as in bacteria, fungi, insect and mammalian cells. In this cellular environment rotamases are known to have an impact on cell proliferation and mitosis, respectively. Because of this, rotamase inhibitors may be used for the treatment of a wide variety of disorders involving cell cycle regulation, both procaryotic and eucaryotic cell cycle regulation. The term "treatment" as used herein comprises both treatment and prevention of a disease. It also comprises follow-up treatment of a disease. Follow-up treatment is realized upon a treatment of a disease using compounds preferably different from the one according to the present invention. For example, after stimulating the growth of a cell, tissue or the like by the application of a respective compound such as, e. g., erythropoietin, it might be necessary to stop an overshooting reaction of cell proliferation which may be obtained using the compounds according to the present invention.

In a further aspect the present invention is related to the use of the compounds according to the present invention as a medicament and for the manufacture of a medicament, respectively. It is to be understood that any of the compounds according to the present invention can be used for the treatment of or for the manufacture of a medicament for the treatment of any of the diseases disclosed herein, irrespective of the mode of action or the causative agent involved as may be specified herein. Of Course, it may particularly be used for any form of such disease where the particular causative agent is involved. Causative agent as used herein also means any agent which is observed in connection with the particular disease described and such agent is not necessarily causative in the sense that is causes the observed diseases or diseased condition.

In an embodiment the medicament is for the treatment or prevention of a disease, whereby the disease involves an undesired cell proliferation.

This use of the compounds according to the present invention is based on the fact that the compounds according to the present invention are suitable to inhibit undesired cell proliferation. Undesired cell proliferation comprises the undesired cell proliferation of procaryotic cells as well as undesired cell proliferation of eucaryotic cells. The term undesired

cell proliferation also covers the phenomenon of abnormal cell proliferation, abnormal mitosis and undesired mitosis. Abnormal cell proliferation means any form of cell proliferation which occurs in a manner different from the normal cell proliferation. Normal cell proliferation is a cell proliferation observed under normal circumstances by the majority of cells and organisms, respectively. The same basic definition applies to abnormal mitosis.

More particularly, undesired cell proliferation and undesired mitosis mean a proliferation and a mitosis, respectively, which may be either a normal or an abnormal cell proliferation, however, in any case it is not a cell proliferation or mitosis which is desired. Desired may thus be defined by an individual such as a human being and in particular a physician, and defined within certain boundaries whereby the boundaries as such may reflect the extent of proliferation and mitosis, respectively, observed under usual conditions or in the majority of cells and organisms, respectively, or may be arbitrarily fixed or defined. Cell proliferation as used herein refers preferably to the proliferation of cells forming the organism to be treated or to which a compound according to the present invention shall be administered which is also referred to herein as the first organism. Cell proliferation as used herein also means the proliferation of cells which are different from the cells forming a first organism or species but are the cells forming a second organism or second species. Typically, the second organism enters in or has a relationship with the first organism. Preferably, the first organism is a human being or an animal or plant, also referred to herein as patient, and the second organism is a parasite and pathogen, respectively, to said first organism. Mitosis as used herein, preferably means the cell division of cells being subject to said cell proliferation whereby even more preferably mitosis is the process of cell division whereby a complete set of chromosomes is distributed to the daughter cells.

Without wishing to be bound by any theory, it seems that the compounds according to the present invention act on cells and thus influence their proliferation and mitosis, respectively, by being inhibitors to some enzymatic activity. Preferably, the inhibition is reversible. This activity is shown by the compounds according to the present invention with regard to bacteria, fungi, insect and mammalian cells.

Because of this, the compounds according to the present invention may be used for the treatment of a wide variety of disorders involving cell cycle regulation, both procaryotic and

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eucaryotic cell cycle regulation. The term "treatment" as used herein comprises both treatment and prevention of a disease. It also comprises follow-up treatment of a disease. Follow-up treatment is realized upon a treatment of a disease using compounds preferably different from the one according to the present invention. For example, after stimulating the growth of a cell, tissue or the like by the application of a respective compound such as, e. g., erythropoietin, it might be necessary to stop an overshooting reaction of cell proliferation which may be obtained using the compounds according to the present invention.

By "reversible" herein is meant that the inhibitor binds non-covalently to the respective enzyme, and is to be distinguished from irreversible inhibition. See Walsh, Enzymatic Reaction Mechanisms, Freeman & Co., N.Y., 1979. "Reversible" in this context is a term understood by those skilled in the art. Preferably the compounds according to the present invention are competitive inhibitors, that is, they compete with substrate in binding reversibly to the enzyme, with the binding of inhibitor and substrate being mutually exclusive.

In a preferred embodiment of the compounds according to the present invention the dissociation constant for inhibition of the enzyme(s) with the inhibitor, i. e. the compound according to the present invention, generally referred to and characterized by those in the art as  $K_i$ , is at most about 100  $\mu$ M. By the term "binding constant" or "dissociation constant" or grammatical equivalents herein is meant the equilibrium dissociation constant for the reversible association of inhibitor with enzyme. The dissociation constants are defined and determined as described below. The determination of dissociation constants is known in the art. For example, for reversible inhibition reactions such as those of the present invention, the reaction scheme is as follows:

E+I 
$$\stackrel{k_1}{=}$$
 E\*I (Equation 1)

The enzyme (E) and the inhibitor (I) combine to give an enzyme-inhibitor complex (E\*I). This step is assumed to be rapid and reversible, with no chemical changes taking place; the enzyme and the inhibitor are held together by non-covalent forces. In this reaction,  $k_1$  is the

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second order rate constant for the formation of the E\*I reversible complex.  $k_2$  is the first order rate constant for the dissociation of the reversible E\*I complex. In this reaction, Ki = $k_2/k_1$ .

The measurement of the equilibrium constant K<sub>i</sub> proceeds according to techniques well known in the art. For example, assays generally use synthetic chromogenic or fluorogenic substrates. The respective K<sub>i</sub> values may be estimated using the Dixon plot as described by Irwin Segel in Enzyme Kinetics: Behavior and analysis of rapid equilibrium and steady-state enzyme systems, 1975, Wiley-Interscience Publication, John Wiley & Sons, New York, or for competitive binding inhibitors from the following calculation:

$$1-(v_i/v_o)=[I]/[I]+K_i (1+([S]/K_m)))$$
 (Equation 2)

wherein  $v_0$  is the rate of substrate hydrolysis in the absence of inhibitor, and  $v_i$  is the rate in the presence of competitive inhibitor.

The compounds according to the present invention may be easily screened for their efficacy in relation to the various uses disclosed herein

By a "labelled compound according to the present invention" herein is meant a compound according to the present invention that has at least one element, isotope or chemical compound attached to enable the detection of the compound or the compound bound to a target such as an enzyme. In general, labels as used herein, fall into three classes: a) isotopic labels, which may be radioactive or heavy isotopes; b) immune labels, which may be antibodies or antigens; and c) colored or fluorescent dyes. The labels may be incorporated into the compound at any position. Examples of useful labels include <sup>14</sup>C, <sup>13</sup>C, <sup>15</sup>N, <sup>3</sup>H, biotin, and fluorescent labels as are well known in the art.

As used herein, the term "disease" describes any disease, diseased condition or pathological condition. Such disease may also be defined as abnormal condition. Also, in case of a pathogen, disease means a condition where a pathogen or an unwanted organism is present or present in a concentration or compartment where it is undesired and thus subject to reduction in numbers, removal, elimination and/or destruction by using the compounds according to the present invention.

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The compounds according to the present invention may be used as a medicament and for the manufacture of a medicament, respectively, whereby the medicament is for the treatment of cell proliferative disorders and any of the diseases specified herein. Cell proliferated disorders as used herein, typically involve an abnormal cell proliferation, an undesired cell proliferation, an abnormal mitosis and/or an undesired mitosis.

Cell proliferative disorders contemplated for treatment using the compounds according to the present invention and for the methods disclosed herein include also disorders characterized by unwanted or undesired, inappropriate or uncontrolled cell growth. Preferably, the disease is selected from the group comprising neurodegenerative diseases, stroke, inflammatory diseases, immune based disorders, infectious diseases, heart diseases, fibrotic disorders, cardiovascular diseases and cell proliferative diseases. Rotamases comprise families of ubiquitous and highly conserved enzymes who have been reported to play important roles in biological processes like protein folding, proteolysis, protein dephosphorylation, peptide transport function, cell cycle regulation, protein synthesis. Furthermore various isomerases have been shown to have regulatory functions as stable or dynamic part of heterooligomeric complexes containing physiologically relevant proteins e.g. hormone receptors, ion channels, kinases, and growth factor receptors.

Preferably, the neurodegenerative disease is selected from the group comprising Alzheimer's disease, Huntington's disease, Parkinson's disease, peripheral neuropathy, progressive supranuclear palsy, corticobasal degeneration, frontotemporal dementia, synucleinopathies, multiple system atrophy, amyotrophic lateral atrophy, prion diseases and motor neuron diseases.

The compounds according to the present invention are additionally useful in inhibiting cell cycle (mitosis) or cell division in pathogenic organisms and are, therefore, useful for treating infectious diseases.

In a preferred embodiment the infectious is selected from the group comprising fungal, viral, bacterial and parasite infection.

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Fungal infections contemplated for treatment using the compounds and methods according to the present invention include systemic fungal infections, dermatophytoses and fungal infections of the genito-urinary tract. Fungal infections, preferably systemic fungal infections, include those caused by Histoplasma, Coccidioides, Cryptococcus, Blastomyces, Paracoccidioides, Aspergillus, Nocardia, Sporothrix, Rhizopus, Absidia, Mucor, Hormodendrum, Phialophora, Rhinosporidium, and the like. Dermatophyte infections include those caused by Microsporum, Trichophyton, Epidermophyton, Candida, Pityrosporum, and the like. Fungal disorders of the genito-urinary tract include infections caused by Candida, Cryptococcus, Aspergillus, Zygomycodoides, and the like. Infection by such organisms causes a wide variety of disorders such as ringworm, thrush or candidiasis, San Joaquin fever or Valley fever or coccidiodomycosis, Gilchrist's disease or blastomycosis, aspergillosis, cryptococcosis, histioplasmosis, paracoccidiomycosis, zygomycosis, mycotic keratitis, nail hair and skin disease, Lobo's disease, lobomycosis, chromoblastomycosis, mycetoma, and the like. These infections can be particularly serious, and even fatal, in patients with a depressed immune system such as organ transplant recipients and persons with acquired immunodefficiency syndrome (AIDS). Insofar a patient group which can be treated using the inhibitors according to the present invention are persons with AIDS, particularly those suffering from any of the infectious diseases described herein.

In a further embodiment the bacterial infection is selected from the group comprising infections caused by both Gram-positive and Gram-negative bacteria, including infections caused by Staphylococcus, Clostridium, Streptococcus, Enterococcus, Diplococcus, Hemophilus, Neisseria, Erysipelothricosis, Listeria, Bacillus, Salmonella, Shigella, Escherichia, Klebsiella, Enterobacter, Serratia, Proteus, Morganella, Providencia, Yersinia, Camphylobacter, Mycobacteria, Helicobacter, Legionalla, Nocardia and the like.

In a preferred embodiment the bacterial infection causes a wide variety of diseases. Said disorders are selected, among others, from the group comprising pneumonia, diarrhea, dysentery, anthrax, rheumatic fever, toxic shock syndrome, mastoiditis, meningitis, gonorrhea, typhoid fever, brucellis, Lyme disease, gastroenteritis, tuberculosis, cholera, tetanus and bubonic plague.

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In another embodiment the disease is a viral infection, more particularly a viral infection caused by a virus selected from the group comprising retrovirus, HIV, Papilloma virus, Polio virus, Epstein-Barr, Herpes virus, Hepatitis virus, Papova virus, Influenza virus, Rabies, JC, encephalitis causing virus, hemorrhagic fever causing virus such as Ebola Virus and Marburg Virus.

In a further embodiment the parasite infection is selected from the group comprising infections caused by Trypanosoma, Leishmania, Trichinella, Echinococcus, Nematodes, Classes Cestoda, Trematoda, Monogenea, Toxoplasma, Giardia, Balantidium, Paramecium, Plasmodium or Entamoeba.

The disease may further be a cell proliferative disorder which preferably is selected from the group characterized by unwanted, inappropriate or uncontrolled cell growth. Particular examples include cancer, fibrotic disorders, non-neoplastic growths. The neoplastic cell proliferative disorder is preferably selected from the group comprising solid tumors, and hematopoeitic cancers such as lymphoma and leukemia.

More preferably, the solid tumor is selected from the group comprising carcinoma, sarcoma, osteoma, fibrosarcoma, and chondrosarcoma.

More preferably, the cell proliferative disorder is selected from the group comprising breast cancer, prostate cancer, colon cancer, brain cancer, lung cancer, pancreatic cancer, gastric cancer, bladder cancer, kidney cancer and head and neck cancer. Preferably, the lung cancer is non-small lung cancer and small lung cancer.

In case the disease is a non-neoplastic cell proliferative disorder, it is preferably selected from the group comprising fibrotic disorder. Preferably, the fibrotic disorder is fibrosis.

The disease may also be a non-neoplastic cell proliferative disorder which is selected from the group comprising prostatic hypertrophy, preferably benign prostatic hypertrophy, endometriosis, psoriasis, tissue repair and wound healing.

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Fibrotic disorders which may be treated using the compounds according to the present invention are generally characterized by inappropriate overproliferation of non-cancerous fibroblasts. Examples thereof include fibromyalgia, fibrosis, more particularly cystic, hepatic, idopathic pulmonary, and pericardial fibrosis and the like, cardiac fibromas, fibromuscular hyperplasia, restenosis, atherosclerosis, fibromyositis, and the like.

In another embodiment the immune based and/or inflammatory disease is an autoimmune disease or autoimmune disorder. In a further embodiment, the immune based and/or inflammatory disease is selected from the group comprising rheumatoid arthritis, glomerulonephritis, systemic lupus erythematosus associated glomerulonephritis, irritable bowel syndrome, bronchial asthma, multiple sclerosis, pemphigus, pemphigoid, scleroderma, myasthenia gravis, autoimmune haemolytic and thrombocytopenic states, Goodpasture's syndrome, pulmonary hemorrhage, vasculitis, Crohn's disease, and dermatomyositis.

In a further preferred embodiment the immune based and/or inflammatory disease is an inflammatory condition.

In a still further embodiment the immune based and/or inflammatory disease is selected from the group comprising inflammation associated with burns, lung injury, myocardial infarction, coronary thrombosis, vascular occlusion, post-surgical vascular reocclusion, artherosclerosis, traumatic central nervous system injury, ischemic heart disease and ischemia-reperfusion injury, acute respiratory distress syndrome, systemic inflammatory response syndrome, multiple organ dysfunction syndrome, tissue graft rejection and hyperacute rejection of transplanted organs.

It is also within the present invention that the compounds according to the present invention may be used for the treatment of a patient suffering from a disease or diseased condition as defined above. Such treatment comprises the administration of one or several of the compounds according to the present invention or a medicament or pharmaceutical composition described herein.

Toxicity and therapeutic efficacy of a compound can be determined by standard pharmaceutical procedures in cell culture or experimental animals. Cell culture assays and

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animal studies can be used to determine the  $LD_{50}$  (the dose lethal to 50% of a population) and the  $ED_{50}$  (the dose therapeutically effective in 50% of a population). The dose ratio between toxic and therapeutic effects is the therapeutic index, which can be expressed as the ratio  $LD_{50}/ED_{50}$ . Compounds which exhibit large therapeutic indices are preferred. The data obtained from these cell culture assays and animal studies can be used in formulating a range of dosages suitable for use in humans. The dosage may vary within this range depending upon a variety of factors, e.g., the dosage form employed, the route of administration utilized, the condition of the subject, and the like

For any compound according to the present invention, the therapeutically effective dose can be estimated initially from cell culture assays by determining an IC<sub>50</sub> (i.e., the concentration of the test substance which achieves a half-maximal inhibition of cell proliferation). A dose can then be formulated in animal models to achieve a circulating plasma concentration range that includes the IC<sub>50</sub> as determined in cell culture. Such information can be used to more accurately determine useful doses in humans. Levels in plasma may be measured, for example by HPLC or LC/MS.

It should be noted that the attending physician would know how to and when to terminate, interrupt, or adjust administration due to toxicity, to organ dysfunction, and the like. Conversely, the attending physician would also know to adjust treatment to higher levels if the clinical response were not adequate (precluding toxicity). The magnitude of an administered dose in the management of the disorder of interest will vary with the severity of the condition to be treated, with the route of administration, and the like. The severity of the condition may, for example, be evaluated, in part, by standard prognostic evaluation methods. Further, the dose and perhaps dose frequency will also vary according to the age, body weight, and response of the individual patient. Typically, the dose will be between about 1-10 mg/kg of body weight. About 1 mg to about 50 mg will preferably be administered to a child, and between 25 mg and about 1000 mg will preferably be administered to an adult.

A program comparable to that discussed above may be used in veterinary medicine. The exact dose will depend on the disorder to be treated and will be ascertainable by one skilled in the art using known techniques.

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Depending on the specific conditions to be treated, such compounds may be formulated and administrated systemically or locally. Techniques for formulation and administration may be found in "Remington's Pharmaceutical Sciences", 1990, 18<sup>th</sup> ed., Mack Publishing Co., Easton, PA. The administration of a compound according to the present invention can be done in a variety of ways, including, but not limited to, orally, subcutaneously, intravenously, intranasally, transdermally, intraperitoneally, intramuscularly, intrapulmonary, vaginally, rectally, or intraocularly, just to name a few. In some instances, for example, in the treatment of wounds and inflammation, the compound according to the present invention may be directly applied as a solution or spray.

In a further aspect the present invention is related to a medicament or a pharmaceutical composition comprising at least one active compound and at least one pharmaceutically acceptable carrier, excipient or diluent. As used herein, the active compound is a compound according to the present invention, a pharmaceutically salt or base thereof or a prodrug thereof, if not indicated to the contrary.

For injection, compounds of the invention may be formulated in aqueous solution, preferably in physiologically compatible buffers such as Hank's solution, Ringer's solution, or physiologically saline buffer. For transmucosal administration, penetrants appropriate to the barrier to be permeated are used in the formulation. Such penetrants are generally known in the art.

The use of pharmaceutical acceptable carriers to formulate the compounds according to the present invention into dosages or pharmaceutical compositions suitable for systemic administration is within the scope of the present invention. With proper choice of carrier and suitable manufacturing practice, the compositions of the present invention, in particular those formulated as solutions, may be administered parenterally, such as by intravenous injection. The compounds can be readily formulated using pharmaceutically acceptable carriers well known in the art into dosages suitable for oral administration. Such carriers enable the compounds according to the present invention to be formulated as tablets, pills, capsules, dragees, liquids, gels, syrups, slurries, suspensions and the like, for oral ingestion by a subject to be treated.

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Compounds according to the present invention or medicaments comprising them, intended to be administered intracellularly may be administered using techniques well known to those of ordinary skill in the art. For example, such agents may be encapsulated into liposomes, then administered as described above. Liposomes are spherical lipid bilayers with aqueous interiors. All molecules present in an aqueous solution at the time of liposome formation are incorporated into the aqueous interior. The liposomal contents are both protected from the external microenvironment and, because liposomes fuse with cell membranes, are efficiently delivered into the cell cytoplasm. Delivery systems involving liposomes are disclosed in International Patent Publication No. WO 91/19501, as well as U.S. Patent No. 4,880,635 to Janoff et al. The publications and patents provide useful descriptions of techniques for liposome drug delivery and are incorporated by reference herein in their entirety.

Pharmaceutical compositions comprising a compound according to the present invention for parenteral administration include aqueous solutions of the active compound(s) in water-soluble form. Additionally, suspensions of the active compounds may be prepared as appropriate oily injection suspensions. Suitable lipophilic solvents or vehicles include fatty oils such as sesame oil or castor oil, or synthetic fatty acid esters, such as ethyl oleate or triglycerides, or liposomes. Aqueous injections suspensions may contain compounds which increase the viscosity of the suspension, such as sodium carboxymethyl cellulose, sorbitol, dextran, or the like. Optionally, the suspension may also contain suitable stabilizers or agents which increase the solubility of the compounds to allow for the preparation of highly concentrated solutions.

Pharmaceutical compositions comprising a compound according to the present invention for oral use can be obtained by combining the active compound(s) with solid excipient, optionally grinding the resulting mixture, and processing the mixture of granules, after adding suitable auxiliaries, if desired, to obtain tablets or dragee cores.

Suitable excipients are, in particular, fillers such as sugars, including lactose, sucrose, mannitol, sorbitol, and the like; cellulose preparations, such as, for example, maize starch wheat starch, rice starch, potato starch, gelatin, gum tragacanth, methyl cellulose, hydroxypropylmethyl cellulose, sodium carboxymethyl cellulose, polyvinylpyrrolidone (PVP) and the like, as well as mixtures of any two or more thereof. If desired, disintegrating agents

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may be added, such as cross-linked polyvinyl pyrrolidone, agar, alginic acid or a salt thereof such as sodium alginate, and the like.

Dragee cores as a pharmaceutical composition comprising a compound according to the present invention are provided with suitable coatings. For this purpose, concentrated sugar solutions may be used, which may optionally contain gum arabic, talc, polyvinyl pyrrolidone, carbopol gel, polyethylene glycol, titanium dioxide, lacquer solutions, suitable organic solvents or solvent mixtures, and the like. Dyestuffs or pigments may be added to the tablets or dragee coatings for identification or to characterize different combinations of active compound doses.

Pharmaceutical preparations comprising a compound according to the present invention which can be used orally include push-fit capsules made of gelatin, as well as soft, sealed capsules made of gelatin and a plasticizer, such as glycerol or sorbitol. The push-fit capsules can contain the active ingredients in admixture with filler such as lactose, binders such as starches and/or lubricants such as talc or magnesium stearate and, optionally, stabilizers. In soft capsules, the active compounds may be dissolved or suspended in suitable liquids, such as fatty oils, liquid paraffin, or liquid polyethylene glycols. In addition, stabilizers may be added.

A "patient" for the purposes of the present invention, i. e. to whom a compound according to the present invention or a pharmaceutical composition according to the present invention is administered, includes both humans and other animals and organisms. Thus the compounds, pharmaceutical compositions and methods are applicable to or in connection with both human therapy and veterinary applications including diagnostic(s), diagnostic procedures and methods as well as staging procedures and methods. For example, the veterinary applications include, but are not limited to, canine, bovine, feline, porcine, caprine, equine, and ovine animals, as well as other domesticated animals including reptiles, such as iguanas, turtles and snakes, birds such as finches and members of the parrot family, lagomorphs such as rabbits, rodents such as rats, mice, guinea pigs and hamsters, amphibians, fish, and arthropods. Valuable non-domesticated animals, such as zoo animals, may also be treated. In the preferred embodiment the patient is a mammal, and in the most preferred embodiment the patient is human.

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The pharmaceutical composition according to the present invention comprises at least one compound according to the present invention in a form suitable for administration to a patient. Preferably, a compound according to the present application is in a water soluble form, such as being present as a pharmaceutically acceptable salt, which is meant to include both acid and base addition salts which are also generally referred to herein as pharmaceutically acceptable salts. "Acid addition salt", and more particularly "pharmaceutically acceptable acid addition salts" refers to those salts that retain the biological effectiveness of the free bases and that are not biologically or otherwise undesirable, formed with inorganic acids such as hydrochloric acid, hydrobromic acid, sulfuric acid, nitric acid, phosphoric acid and the like, and organic acids such as acetic acid, propionic acid, glycolic acid, pyruvic acid, oxalic acid, maleic acid, malonic acid, succinic acid, fumaric acid, tartaric acid, citric acid, benzoic acid, cinnamic acid, mandelic acid, methanesulfonic acid, ethanesulfonic acid, p-toluenesulfonic acid, salicylic acid and the like. "Base addition salts" and more particularly "pharmaceutically acceptable base addition salts" include those derived from inorganic bases such as sodium, potassium, lithium, ammonium, calcium, magnesium, iron, zinc, copper, manganese, aluminum salts and the like. Particularly preferred are the ammonium, potassium, sodium, calcium, and magnesium salts. Salts derived from pharmaceutically acceptable organic nontoxic bases include salts of primary, secondary, and tertiary amines, substituted amines including naturally occurring substituted amines, cyclic amines and basic ion exchange resins, such as isopropylamine, trimethylamine, diethylamine, triethylamine, tripropylamine, and ethanolamine. The pharmaceutical compositions according to the present invention may also include one or more of the following: carrier proteins such as serum albumin; buffers; fillers such as microcrystalline cellulose, lactose, corn and other starches; binding agents; sweeteners and other flavoring agents; coloring agents; and polyethylene glycol. Additives are well known in the art, and are used in a variety of formulations.

The compounds according to the present invention are, in a further embodiment, administered to a subject either alone or in a pharmaceutical composition where the compound(s) is mixed with suitable carriers or excipient(s). In treating a subject, a therapeutically effective dose of compound (i.e. active ingredient) is administered. A therapeutically effective dose refers to that amount of the active ingredient that produces amelioration of symptoms or a prolongation

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of survival of a subject which can be determined by the one skilled in the art doing routine testing.

On the other hand, the compounds according to the present invention may as such or contained in a pharmaceutical composition according to the present invention be used in drug potential applications.

For example, therapeutic agents such as antibiotics or antitumor drugs can be inactivated through the catalytic action of endogenous enzymes, thus rendering the administered drug less effective or inactive. Accordingly, the compound(s) according to the present invention may be administered to a patient in conjunction with a therapeutic agent in order to potentiate or increase the activity of the drug. This co-administration may be by simultaneous administration, such as a mixture of the compound(s) according to the present invention and the drug, or by separate simultaneous or sequential administration.

According to the present invention the compounds disclosed herein, referred to as compounds according to the present invention, may be used as a medicament or for the manufacture of medicament or in a method of treatment of a patient in need thereof. Insofar any of these compounds constitute a pharmaceutical compound. The use of this kind of compound also comprises the use of pharmaceutically acceptable derivatives of such compounds.

In addition, the compounds according to the present invention may be transformed upon application to an organism such as a patient, into the pharmaceutically active compound. Insofar the compounds according to the present invention may be prodrugs which, however, are nevertheless used for the manufacture of the medicaments as disclosed herein given the fact that at least in the organism they are changed in a form which allows the desired.

It is to be understood that any of the pharmaceutical compositions according to the present invention may be used for any of the diseases described herein.

The pharmaceutical compositions according to the present invention may be manufactured in a manner that is known as such, e.g., by means of conventional mixing, dissolving,

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granulating, dragee-mixing, levigating, emulsifying, encapsulating, entrapping, lyophilizing, processes, or the like.

In a further aspect of the present invention the compounds of the present invention may be used as insecticides as they may prevent cell cycle mitosis in insect cells and thus can be used to control the growth and proliferation of a variety of insect pests. This aspect of the present invention has important applications in agriculture, such as in the field, in the storage of agricultural products and the like. Additionally, the compounds according to the present invention are useful for controlling insect populations, preferably in places inhabited by men, such as homes, offices and the like.

Any of the compounds according to the present invention containing one or more asymmetric carbon atoms may occur as racemates and racemic mixtures, single enantiomers, diastereomeric mixtures and individual diastereomers. All such isomeric forms of these compounds are expressly included in the present invention. Each stereogenic carbon may be in the R or S configuration, or a combination of configurations.

It shall be understood by the one of ordinary skill in the art that all compounds of the invention are preferably those which are chemically stable. This applies to any of the various uses of the compounds according to the present invention disclosed herein.

In determining the suitability of any of the compounds according to the present applications for the various uses, besides the particular use-specific profile to be met by such a compound, also it has to be checked whether it is stable to proteolytic degradation. The resistance of the compound used as a pharmaceutical may be tested against a variety of non-commercially available proteases in vitro to determine its proteolytic stability. Promising candidates may then be routinely screened in animal models, for example using labelled inhibitors, to determine the *in vivo* stability and efficacy. In any of the aforementioned uses the compound may be present in a crude or purified form. Methods for purifying the compounds according to the present invention are known to the one skilled in the art.

The problem underlying the present invention is also solved by the technical teaching according to the attached independent claims. Preferred embodiments thereof may be taken from the dependent claims.

The invention is now further illustrated by reference to the following figures and examples from which further advantages, features and embodiments may be taken. It is understood that these examples are given for purpose of illustration only and not for purpose of limitation. All references cited herein are incorporated by reference.

- Fig. 1 shows FACS results of compound 703,
- Fig. 2 show a FACS analysis of the effect of various compounds on HL 60 cells as a measure for the apoptotic activity of the compounds; and
- Fig. 3 shows fluorescence microscope photographs of DAPI stained HeLa cells after treatment with various compounds

# Example 1: Material and Methods

In order that the invention herein described may be more fully understood, the following detailed description is set forth. As used herein, the following abbreviations are used:

Ar is argon;

D is doublet;

DCM is dichloromethane;

DIPEA is N,N-diisopropylethylamine;

DMF is N,N-dimethylformamide;

DMSO is N,N-dimethylsulfoxide;

eq is equivalent;

Et<sub>3</sub>N is triethylamine;

HCl is chlorhydric acid;

HPLC is high performance liquid chromatography;

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h is hour;
Hz is hertz;
m is multiplet;
mL is milliliter;
NaHCO<sub>3</sub> is sodium hydrogencarbonate;
s is singulet;
THF is tetrahydrofuran.

### Method A: Urea formation in solution

Amine salt and DIPEA (1 eq each) or amine (1 eq) was dissolved in dry dioxan and a solution of the isocyanate (1 eq) in DCM or DMSO was added under Ar in one portion. The solution was stirred for 3 h at room temperature. The solution was diluted with 2 ml DCM and scavenger resins (tris-(2-aminoethyl)-amine polystyrene (3 eq), methylisocyanate polystyrene (3 eq) and N-(2-mercaptoethyl)aminomethyl polystyrene (3 eq)) were added to remove unreacted isocyanate, amine and electrophilic impurities respectively. After 18 h at 40°C, the solution was filtered off and the solvent was removed under reduced pressure. The obtained crude ureas were purified by HPLC.

# Method B: Coupling of substituted anilines with sulfonyl chlorides

Aniline (30 mg) and NEt<sub>3</sub> (1.2 eq, 2.2 eq. when HCl salt) were dissolved in dry acetonitrile (0.5 mL). Sulfonyl chloride (1 eq) was dissolved in dry acetonitrile (0.5 mL) and added to the solution. The reaction mixture was stirred under argon for 12 h at 40°C. Tris-(2-aminoethyl)-amine polystyrene (30 mg), (polystyrylmethyl) trimethylammonium bicarbonate (30 mg), N-(2-mercaptoethyl)amino methyl polystyrene (30 mg), and methylisocyanate polystyrene (30 mg) were given to the solution and stirred for additional 12 h at 40°C. After filtration the solvent was removed under reduced pressure. The crude reaction product was purified by preparative HPLC using acetonitrile and water as mobile phase.

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### Method C: Coupling of substituted anilines with acid chlorides

Aniline (30 mg) and NEt<sub>3</sub> (1 eq, 2 eq. when HCl salt) were dissolved at 0°C in dry DCM (0.5 mL) with 10% DMSO. Acid chloride (1 eq) was dissolved at 0°C in dry DCM (0.5 mL) and added to the solution. The reaction mixture was stirred under argon for 2 h while slowly warming up to room temperature. Work up was performed by pouring the reaction mixture with DCM over incubated HYDROMATRIX layers. 2 mL basic layer (saturated NaHCO<sub>3</sub> solution 2 ml/g HYDROMATRIX), 2 mL acidic layer (2M HCl 2 ml/g HYDROMATRIX), and 2 mL of dry HYDROMATRIX layer in a 10 ml syringe were used. The solvent was removed under reduced pressure. The crude reaction product was purified by preparative HPLC using acetonitrile and water as mobile phase.

## Method D: Reductive amination of aldehydes with hydroxyl anilines

Amine hydrochloride (0.11 mmol, 1 eq), aldehyde (0.11 mmol, 1 eq), and DIPEA (0.11 mmol, 1 eq) were dissolved in anhydrous THF (1 mL), and molecular sieves 4Å (10 mg) was shaking for 1.5 h at room temperature, After solution. added to (polystyrylmethyl)trimethylammonium cyanoborohydride (4.3 mmol/g, 0.22 mmol) was added to the reaction mixture. After shaking for 8 h at room temperature, 4-(3 mmol/g, 0.22 mmol), 3-(4polystyrene benzyloxybenzaldehyde (hydrazinosufonyl)phenyl)propionyl AM resin (1.5 mmol/g, 0.22 mmol), and N-(2mercaptoethyl)aminomethyl polystyrene (2.1 mmol/g, 0.22 mmol) were added, after which the reaction mixture was shaken at room temperature for 18 h. Filtration, washing with DCM, and evaporation of the solvent in vacuo afforded the crude product, which was purified by reversed phase HPLC.

# Method E: Condensation of amines with hydroxyl carboxylic acids

1-Ethyl-3(3'-dimethylaminophropyl)carbodiimide hydrochloride (0.15 mmol, 1.36 eq), hydroxyl carboxylic acid (0.15 mmol, 1.36 eq), and 1-hydroxy-7-azabenzotriazole (0.15 mmol, 1.36 eq) were dissolved in DMF (0.7 mL). After shaking for 30 min at room temperature, a solution of amine (0.11 mmol) in DMF (0.7 mL) was added to the reaction mixture. After shaking for 2 h at room temperature, amine (0.22 mmol) was added, after which the reaction mixture was shaken at 60 °C overnight. Then the solvent was evaporated in vacuo, and the residue was dissolved in DCM (7 mL). HYDROMATRIX™ (0.3 g) which

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was previously treated with HCl (2N, 0.6 mL) was added to the solution, and the mixture was shaken for 30 min. Filtration, washing with DCM, and evaporation of the solvent in vacuo afforded the crude product, which was purified by reversed phase HPLC.

### Method F: Carbamate formation in solution

Amine or amine salt (1 eq) and sodium bicarbonate (1 or 2 eq) were dissolved in a mixture of MeOH / H<sub>2</sub>O (3:1). The mixture was treated with chloroformate (1 eq), which was added in three portions over 10 minutes. After 30 minutes at room temperature, the precipitating product was collected by filtration and washed with water. The obtained crude carbamates were purified by HPLC.

#### Method G: Carbamate formation in solution

To an ice cooled mixture of amine or amine salt (1 eq) and DIPEA (1.1 eq or 2.2 eq) in dry DCM was added an ice cooled solution of chloroformate (1.1 eq) in DCM in one portion. After 1.5-8 h at room temperature the solvent was removed under reduced pressure. The obtained crude carbamates were purified by HPLC.

#### Method H: Carbamate formation in solution

To a mixture of amine or amine salt (1 eq) and sodium bicarbonate (1 or 2.5 eq) in dry DCM was added chloroformate (1 eq) in one portion. After 4 hours at room temperature the sodium bicarbonate was filtered off and the solvent was removed under reduced pressure. The obtained crude carbamates were purified by HPLC.

#### Method I: Thiourea formation in solution

Amine salt and DIPEA (1 eq each) or amine (1 eq) was dissolved in dry dioxan and a solution of the thioisocyanate (1 eq) in DCM or DMSO was added under Ar in one portion. The solution was stirred for 3 h at room temperature. The solution was diluted with 2 ml DCM and scavenger resins (tris-(2-aminoethyl)-amine polystyrene (3 eq), methylisocyanate polystyrene (3 eq) and N-(2-mercaptoethyl)aminomethyl polystyrene (3 eq)) were added to remove

unreacted isocyanate, amine and electrophilic impurities respectively. After 18 h at 40°C, the solution was filtered off and the solvent was removed under reduced pressure. The obtained crude thioureas were purified by HPLC.

### Method J: Synthesis of (3-amino-5-chloro-4-hydroxy-phenyl)-ureas.

Isocyanate (5.0 mmol) was added to a stirred solution of 4-Amino-2-chloro-phenol (5.0 mmol) in anhydrous CH<sub>2</sub>Cl<sub>2</sub> (23 mL) and THF (4 mL) at room temperature. After stirring for 12 h, the solvent was evaporated in vacuo. The residue was then dissolved in HOAc (95 mL) and added in one single portion to a stirred solution of NaNO<sub>2</sub> (1.17 g, 17.0 mmol) in H<sub>2</sub>O (8.4 mL). The flask was sealed with a stopper and the reaction mixture was stirred for 1.5 min at room temperature. The reaction was stopped by the addition of saturated aqueous NaHCO<sub>3</sub> (190 mL). After stirring for 10 min at room temperature, the yellow precipitate was filtered, washed with H<sub>2</sub>O (3 x 30 mL), and dried in vacuo. The yellow residue was then dissolved in a mixture of toluene (75 mL) and MeOH (90 mL). Raney nickel (0.5 g) was washed with MeOH (5 x 10 mL) and added to the reaction mixture. Then the reaction mixture was vigorously stirred under a hydrogen atmosphere at 1 bar at room temperature for 2 h. Filtration through a pad of Celite and evaporation of the solvent afforded the aniline, which was converted into the corresponding diureas by method A, the corresponding amilines by method D, the corresponding sulfonamides by method I.

Method K: Synthesis of (5-benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-ureas, (5-benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-thioureas, (3-benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-ureas, (3-benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-thioureas, (5-benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-amides, and (3-benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-amides.

3-Chloro-2-hydroxy-5-nitro-benzoic acid or 3-chloro-4-hydroxy-5-nitro-benzoic acid (0.41 g, 1.9 mmol) was dissolved in polyphosphoric acid (12.3 g) at 110 °C. 2-Aminothiophenol (0.36 mg, 2.9 mmol) was added and the resulting solution was stirred at 110 °C for 5 h. After cooling, ammonia (35% in  $H_2O$ , 12 mL) was added to the reaction mixture. The precipitate was filtered, washed with  $H_2O$  (3 x 10 mL) and dried in vacuo. The residue was then

dissolved in a mixture of MeOH (30 mL) and THF (70 mL). Raney nickel (0.5 g) was washed with MeOH (5 x 10 mL) and added to the reaction mixture. Then the reaction mixture was vigorously stirred under a hydrogen atmosphere at 1 bar at room temperature for 1 h. Filtration through a pad of Celite and evaporation of the solvent afforded the aniline, which was converted into the corresponding ureas by method A, the corresponding amides by method C or E, or the corresponding thioureas by method I.

# Method L: Synthesis of (3-amino-5-chloro-4-hydroxy-phenyl)-amides.

Acyl chloride (5.0 mmol) was added to a stirred solution of 4-Amino-2-chloro-phenol (5.0 mmol) in anhydrous CH<sub>2</sub>Cl<sub>2</sub> (23 mL) and THF (4 mL) at O°C. After stirring for 12 h, the solvent was evaporated in vacuo. The residue was then dissolved in HOAc (95 mL) and added in one single portion to a stirred solution of NaNO<sub>2</sub> (1.17 g, 17.0 mmol) in H<sub>2</sub>O (8.4 mL). The flask was sealed with a stopper and the reaction mixture was stirred for 1.5 min at room temperature. The reaction was stopped by the addition of saturated aqueous NaHCO<sub>3</sub> (190 mL). After stirring for 10 min at room temperature, the yellow precipitate was filtered, washed with H<sub>2</sub>O (3 x 30 mL), and dried in vacuo. The yellow residue was then dissolved in a mixture of toluene (75 mL) and MeOH (90 mL). Raney nickel (0.5 g) was washed with MeOH (5 x 10 mL) and added to the reaction mixture. Then the reaction mixture was vigorously stirred under a hydrogen atmosphere at 1 bar at room temperature for 2 h. Filtration through a pad of Celite and evaporation of the solvent afforded the aniline, which was converted into the corresponding ureas by method A, the corresponding anilines by method C or E, or the corresponding thioureas by method I.

Example 2: 1-Adamantan-1-yl-3-(3,5-dichloro-2-hydroxy-4-methyl-phenyl)-urea

To a solution of 6-amino-2,4-dichloro-3-methyl-phenol hydrochloride (113.5 mg, 1 eq) and DIPEA (48 μL, 1 eq) in dioxan (1.1 mL) was added 1-adamantylisocyanate (88.5 mg, 1 eq) in 580 μL DMSO in one portion. The solution was stirred at room temperature for 3 h. The solution was diluted with 2 mL DCM and scavenger resins (tris-(2-aminoethyl)-amine polystyrene (3 eq), methylisocyanate polystyrene (3 eq) and N-(2-mercaptoethyl)aminomethyl polystyrene (3 eq)) were added. After 18 h at 40°C the solution was filtered off and the solvent was removed under reduced pressure. The crude product was purified by HPLC to obtain 118 mg (64 %) of the title compound as a white powder.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  = 1.62 (s<sub>b</sub>, 6H), 1.92 (s<sub>b</sub>, 6H), 2.05 (s<sub>b</sub>, 3H), 2.29 (s, 3H), 6.79 (s, 1H), 7.95 (s, 1H), 8.15 (s, 1H), 9.82 (s, 1H).

NMR-<sup>13</sup>C (DMSO-d<sub>6</sub>)  $\delta$  = 17.1, 29.3, 36.1, 41.5, 50.3, 116.3, 122.1, 123.8, 124.7, 129.9, 140.6, 154.3; MS (m/z): 369.2 [M+H<sup>+</sup>].

Example 3: 1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-urea

To a solution of 4-amino-2,6-dichloro-phenol (44.5 mg, 1 eq) in dioxan (2.0 mL) was added 2-isocyanato-2,4,4-trimethyl-pentane (38 mg, 1 eq) in one portion. The solution was stirred at room temperature for 3 h. The solution was diluted with 2 mL DCM and scavenger resins (tris-(2-aminoethyl)-amine polystyrene (3 eq), methylisocyanate polystyrene (3 eq) and N-(2-mercaptoethyl)aminomethyl polystyrene (3 eq)) were added. After 18 h at 35°C the solution was filtered off and the solvent was removed under reduced pressure. The crude material was purified by HPLC to obtain 67 mg (81%) of the title compound as a white powder.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  = 0.95 (s, 9H), 1.30 (s, 6H), 1.70 (s, 2H), 2.30 (s, 3H), 6.80 (s, 1H), 8.00 (s, 1H), 8.08 (s, 1H), 9.83 (s<sub>b</sub>, 1H).

NMR- $^{13}$ C (DMSO- $^{13}$ C (DMSO- $^{13}$ C)  $\delta = 29.7, 31.2, 50.5, 53.2, 117.3, 122.4, 134.0, 142.8, 153.9; MS (m/z): 333.2 [M+H<math>^{1}$ ].

Example 4: 2 N-(2-Hydroxy-4-methyl-phenyl)-C-phenyl-methanesulfonamide

The compound was obtained in 32% yield (21.2 mg) using the protocol described in method A.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  = 2.13 (s, 3H), 4.97 (s, 2H), 6.70 (d, 1H, J = 8.2 Hz), 6.78 (s, 1H), 6.83 (d, 1H, J = 8.2 Hz), 7.43 (m, 2H), 7.49 (m, 2H); MS (m/z): 278.1 [M<sup>+</sup>].

Example 5: Propane-2-sulfonic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide

The compound was obtained in 47% yield (22.1 mg) using the protocol described in method B.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  = 2.25 (d, 6H, J = 6.8), 2.27 (s, 3H), 3.97 (hep, 1H, J = 6.8), 5.39 (s, 1H), 6.91 (s, 1H); MS (m/z): 298.1 [MH<sup>+</sup>].

Example 6: N-(3,5-Dichloro-2-hydroxy-phenyl)-2-phenyl-acetamide

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The compound was obtained in 22% yield (11.0 mg) using the protocol described in method C.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  = 3.06 (s, 2H), 7.25 (m, 1H), 7.31 (m, 2H), 7.32 (m, 2H), 7.61 (m, 2H), 9.87 (m, 1H); MS (m/z): 296.2 [MH<sup>+</sup>].

Example 7: N-(3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-N-methyl-2-trifluoromethyl-benzamide

Aniline HCL salt (300 mg, 1.3 mmol) and K<sub>2</sub>CO<sub>3</sub> (500 mg) were dissolved in DMSO (5 mL). CH<sub>3</sub>I (187 mg, 1.3 mmol) was added and the suspension was stirred for 48 h at room temperature. After filtration, the solvent was removed under reduced pressure. The crude reaction product was purified by preparative HPLC using acetonitrile and water as mobile phase to give the *N*-methyl amino phenol derivative (130 mg, 31 %).

The amide was obtained in 56% yield (19.7 mg) using the protocol described in method C. NMR- $^{1}$ H (DMSO-d<sub>6</sub>)  $\delta$  = 2.41 (s, 3H), 3.75 (s, 3H), 7.70–7.85 (m, 4H), 8.05 (d, 1H, J = 5.0); MS (m/z): 377.9 [MH $^{+}$ ].

Example 8: 2,4-Dichloro-3-methyl-6-(3-methyl-benzylamino)-phenol

The compound was obtained in 49 % yield (16 mg) using the protocol described in method D. According to method D.

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NMR- $^{1}$ H (DMSO-d<sub>6</sub>)  $\delta$  2.21 (s, 3 H), 2.27 (s, 3 H), 4.27 (s, 2 H), 5.80 (br s, 1 H), 6.35 (s, 1 H), 7.02-7.24 (m, 4 H), 9.18 (br s, 1 H); MS (m/z): 296.2 [M+H $^{+}$ ].

<u>Example 9</u>: 1-{5-Chloro-3-[2-(4-chloro-phenylsulfanyl)-benzylamino]-2-hydroxy-phenyl}-ethanone

The compound was obtained in 18 % yield (12 mg) using the protocol described in method D. NMR- $^{1}$ H (DMSO- $^{1}$ d<sub>6</sub>)  $\delta$  2.60 (s, 3 H), 4.40 (s, 2 H), 6.24 (d, J = 2.0 Hz, 1H), 6.41 (m, 1H), 7.10 (d, J = 2 Hz, 1H), 7.18-7.24 (m, 2 H), 7.29-7.44 (m, 6 H), 12.66 (s, 1 H); MS: m/z: 418.5 [M+H<sup>+</sup>].

Example 10: 4-Chloro-2-[2-(4-chloro-phenylsulfanyl)-benzylamino]-6-(1-hydroxy-ethyl)-phenol

The compound was obtained in 34 % yield (23 mg) using the protocol described in method D. NMR- $^{1}$ H (DMSO- $^{1}$ d<sub>6</sub>)  $\delta$  1.27 (d, J = 6.4 Hz, 3 H), 4.33 (s, 2 H), 4.97 (q, J = 6.4 Hz, 1 H), 5.96 (d, J = 2.4 Hz, 1 H), 6.47 (d, J = 2.4 Hz, 1 H), 7.19-7.47 (m, 8 H), 8.69 (br. S, 1 H); MS: m/z: 420.7 [M+H<sup>+</sup>].

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Example 11: (3,5-Dichloro-2-hydroxy-phenyl)-carbamic acid phenyl ester

The compound was obtained in 26 % yield (11 mg) using the protocol described in method F. NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$ = 7.25 (m, 3H), 7.43 (m, 2 H), 7.50 (s, 2H) NMR-<sup>13</sup>C (DMSO-d<sub>6</sub>)  $\delta$ = 109.1, 118.8, 121.4, 128.2, 129.4, 132.6, 153.2, 157.3

Example 12: (3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-carbamic acid phenyl ester

The compound was obtained in 31 % yield (24 mg) using the protocol described in method F. NMR- $^{1}$ H (DMSO- $^{1}$ d<sub>6</sub>)  $\delta$ = 2.38 (s, 3 H), 6.76 (m, 3H), 7.15 (m, 3H) NMR- $^{13}$ C (DMSO- $^{13}$ C (DMSO- $^{13}$ d<sub>6</sub>)  $\delta$ = 16.5, 109.1, 115.2, 118.8, 126.7, 128.5, 129.5, 129.7, 139.4, 153.4, 157.4

Example 13: (3,5-Dichloro-2-hydroxy-phenyl)-carbamic acid benzyl ester

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According to method F 2-amino-4,6-dichloro-phenol (25 mg, 1 eq) and phenylchloroformate (23  $\mu$ L, 1 eq) gave 10.9 mg (26 %) of the title compound as a white solid. NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$ = 5.30 (d, 2 H), 7.43 (m, 2 H), 7.25 (m, 2H), 7.50 (s, 2H)

Example 14: (3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-carbamic acid 2-isopropyl-5-methyl-cyclohexyl ester

The compound was obtained in 39% yield (22 mg) using the protocol described in method G. NMR- $^{1}$ H (DMSO-d<sub>6</sub>)  $\delta$  = 0.84-0.90 (m, 3H), 1.22-1.41 (m, 6H), 2.35 (s, 3H), 3.28-3.33 (m, 2H), 4.06 (t, 2H), 7.57 (s, 1H), 8.74 (s, 1H).

Example 15: (3,5-Dichloro-2-hydroxy-phenyl)-carbamic acid 2-isopropyl-5-methyl-cyclohexyl ester

The compound was obtained in 54% yield (44 mg) using the protocol described in method G. NMR- $^{1}$ H (DMSO- $^{1}$ d<sub>6</sub>)  $\delta$  = 0.75 (d, 3H), 0.82-093 (m, 7H), 0.96-1.14 (m, 2H), 1.29-1.53 (m, 2H), 1.59-1.71 (m, 2H), 1.88-2.02 (m, 2H), 4.54 (ddd, 1H), 7.47 (s, 2H), 9.67 (s, 1H), 9.73 (s, 1H)

Example 16: (3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-carbamic acid hexyl ester

The compound was obtained in 21% yield (10 mg) using the protocol described in method G. NMR- $^{1}$ H (DMSO- $^{1}$ d<sub>6</sub>)  $\delta$  = 0.87 (t, 3H), 1.25-1.40 (m, 6H), 1.55-1.66 (m, 2H), 2.35 (s, 3H), 4.06 (t, 2H), 7.56 (s, 1H), 8.74 (s, 1H), 9.73 (s, 1H).

Example 17: (3,5-Dichloro-2-hydroxy-phenyl)-carbamic acid hexyl ester

The compound was obtained in 43% yield (30 mg) using the protocol described in method G. NMR- $^{1}$ H (DMSO-d<sub>6</sub>)  $\delta$  = 0.87 (t, 3H), 1.21-1.40 (m, 6H), 1.54-1.66 (m, 2H), 4.06 (t, 2H), 7.46 (s, 2H), 9.67 (s, 1H), 9.73 (s, 1H).

Example 18: 1-[3-Chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-3-(1,1,3,3-tetramethyl-butyl)-urea

The compound was obtained in 31% yield (16 mg) using the protocol described in method J. NMR- $^{1}$ H (DMSO- $^{1}$ d<sub>6</sub>)  $\delta$  1.06 (s, 9 H), 1.08-1.28 (m, 5 H), 1.35 (s, 6 H), 1.45-1.76 (m, 7 H), 3.30-3.42 (m, 1 H), 6.84 (s, 1 H), 7.24 (s, 1 H), 7.73 (s, 1 H), 8.20 (br. s, 1 H), 8.82 (s, 1 H), 8.97 (s, 1 H), 9.11 (s, 1 H); MS: m/z: 439.2 [M+H<sup>+</sup>].

Example 19: N-[3-Chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-2-nitrobenzenesulfonamide

According to method J 1-(3-amino-5-chloro-4-hydroxy-phenyl)-3-cyclohexyl-urea (19 mg, 67  $\mu$ mol) and 2-nitro-benzenesulfonyl chloride (15 mg, 67  $\mu$ mol) gave N-[3-Chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-2-nitro-benzenesulfonamide (15 mg, 48%). NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  1.05-1.37 (m, 5 H), 1.49-1.83 (m, 5 H), 3.42-3.47 (m, 1 H), 5.94 (d, J = 7.9 Hz, 1 H), 6.99 (d, J = 2.4 Hz, 1 H), 7.46 (d, J = 2.4 Hz, 1 H), 7.78-7.90 (m 2 H), 7.93-8.03 (m, 2 H), 8.27 (s, 1 H), 9.19 (br s, 1 H), 9.70 (s, 1 H); MS: m/z: 469.1 [M+H<sup>+</sup>].

Example 20: 1-(3-Benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-3-cyclohexyl-urea

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According to method K 4-amino-2-benzothiazol-2-yl-6-chloro-phenol (21 mg, 76 µmol) and isocyanato-cyclohexane (9.5 mg, 76 µmol) gave 1-(3-Benzothiazol-2-yl-5-chloro-4-hydroxy-phenyl)-3-cyclohexyl-urea (3.0 mg, 10%).

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  1.09-1.41 (m, 5 H), 1.49-1.87 (m, 5 H), 3.41-3.47 (m, 1H), 6.12 (d, J = 7.8 Hz, 1 H), 7.51 (t, J = 7.8 Hz, 1 H), 7.60 (t, J = 7.1 Hz, 1 H), 7.68 (d, J = 2.4 Hz, 1 H), 8.06 (d, J = 2.4 Hz, 1 H), 8.11 (d, J = 8.3 Hz, 1 H), 8.21 (d, J = 7.3 Hz, 1 H), 8.52 (s, 1 H), 11.92 (s, 1 H); MS: m/z: 402.2 [M+H<sup>+</sup>].

Example 21: 1-(5-Benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-3-(2-trifluoromethyl-phenyl)-thiourea

According to method K 2-Amino-4-benzothiazol-2-yl-6-chloro-phenol (20 mg, 72 μmol) and 1-isothiocyanato-2-trifluoromethyl-benzene (15 mg, 72 μmol) gave 1-(5-benzothiazol-2-yl-3-chloro-2-hydroxy-phenyl)-3-(2-trifluoromethyl-phenyl)-thiourea (12 mg, 35%).

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  7.40-7.56 (m, 3 H), 7.66-7.79 (m, 3 H), 7.92 (d, J = 2.4 Hz, 1 H), 8.03 (d, J = 7.8 Hz, 1 H), 8.12 (d, J = 8.8 Hz, 1 H), 8.68 (br s, 1 H), 9.65 (s, 1 H), 9.94 (s, 1 H), 10.65 (s, 1 H); MS: m/z: 480.0 [M+H<sup>+</sup>].

Example 22: 1-(3,5-Dichloro-2-hydroxy-4-methyl-phenyl)-3-(4-trifluoromethyl-phenyl)-thiourea

The compound was obtained in 57% yield (59 mg) using the protocol described in method I. NMR- $^{1}$ H (DMSO- $^{1}$ d<sub>6</sub>)  $\delta = 2.38$  (s, 3 H), 7.68-7.85 (m, 5 H), 9.43 (s, 1 H), 9.90 (s, 1 H), 10.37 (s, 1 H); MS (m/z): 278.1 [M<sup>+</sup>].

Example 23: 1-Adamantan-1-yl-3-(3,5-dichloro-4-hydroxy-phenyl)-urea

The compound was obtained in 60% yield (35 mg) using the protocol described in method A. NMR- $^{1}$ H (DMSO- $^{1}$ d<sub>6</sub>)  $\delta = 1.60$  (s<sub>b</sub>, 6H), 1.95 (s<sub>b</sub>, 6H), 2.08 (s<sub>b</sub>, 3H), 6.79 (s, 1H), 7.95 (s, 1H), 8.18 (s, 1H), 9.82 (s, 1H).

NMR- $^{13}$ C (DMSO- $^{13}$ C (DMSO- $^{13}$ C)  $\delta = 17.2, 29.5, 36.1, 41.7, 50.3, 116.2, 122.2, 123.8, 124.8, 140.6, 154.3; MS (m/z): 369.2 [M+H<sup>+</sup>].$ 

Example 24: 1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(1,1,3,3-tetramethyl-butyl)-urea

To a solution of 4-amino-2,6-dichloro-phenol (44.5 mg, 1 eq) in dioxan (2.0 mL) was added 2-isocyanato-2,4,4-trimethyl-pentane (38 mg, 1 eq) in one portion. The solution was stirred at room temperature for 3 h. The solution was diluted with 2 mL DCM and scavenger resins (tris-(2-aminoethyl)-amine polystyrene (3 eq), methylisocyanate polystyrene (3 eq) and N-(2mercaptoethyl)aminomethyl polystyrene (3 eq)) were added. After 18 h at 35°C the solution was filtered off and the solvent was removed under reduced pressure. The crude material was purified by HPLC to obtain 67 mg (81%) of the title compound as a white powder.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta = 0.95$  (s, 9H), 1.28 (s, 6H), 1.69 (s, 2H), 5.90 (s, 1H), 7.33 (s, 2H), 8.22 (s, 1H), 9.50 (s<sub>b</sub>, 1H).

NMR-<sup>13</sup>C (DMSO-d<sub>6</sub>)  $\delta$  = 29.9, 31.2, 50.9, 54.2, 117.3, 121.4, 134.0, 142.8, 152.9; MS (m/z): 333.2 [M+H<sup>+</sup>].

Example 25: 1-(3,5-Dichloro-4-hydroxy-phenyl)-3-(4-trifluoromethyl-phenyl)-thiourea

The compound was obtained in 58% yield (34.8 mg) using the protocol described in method I. NMR- $^{1}$ H (DMSO- $^{1}$ G)  $\delta = 6.32$  (m, 2 H), 6.80 (m, 2 H), 7.42 (m, 2 H), MS (m/z): 381.2 [M $^{+}$ ].

Example 26: Propane-2-sulfonic acid (3,5-dichloro-2-hydroxy-4-methyl-phenyl)-amide

The compound was obtained in 40% yield (21 mg) using the protocol described in method B.

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NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta = 2.43$  (d, 6H), 2.51 (s, 3H), 3.97 (m, 1H), 5.43 (s, 1H), 6.8 (s, 1H); MS (m/z): 284.1 [MH<sup>+</sup>].

Example 27: N-(3,5-Dichloro-4-hydroxy-phenyl)-2-phenyl-acetamide

The compound was obtained in 22% yield (11.0 mg) using the protocol described in method C.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  = 3.12 (s, 2H), 7.24 (m, 1H), 7.36 (m, 2H), 7.37 (m, 2H), 7.61 (m, 2H), 9.91 (m, 1H); MS (m/z): 296.2 [MH<sup>+</sup>].

Example 28: 2,6-Dichloro-4-(3-methyl-benzylamino)-phenol

The compound was obtained in 55% yield (15.0 mg) using the protocol described in method D.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  2.26 (s, 3 H), 4.29 (s, 2 H), 5.92 (s, 1 H), 6.50 (s, 1 H), 7.00-7.28 (m, 4 H), 9.20 (s, 1 H); MS (m/z): 282.2 [M+H<sup>+</sup>].

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Example 29: (3,5-Dichloro-4-hydroxy-phenyl)-carbamic acid phenyl ester

The compound was obtained in 49% yield (55.7 mg) using the protocol described in method . F.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  = 7.22 (m, 2H), 7.36 (m, 2 H), 7.50 (s, 2H) NMR-<sup>13</sup>C (DMSO-d<sub>6</sub>)  $\delta$  = 118.5, 121.9, 122.5, 125.5, 129.4, 131.7, 144.7, 150.3, 151.6

Example 30: (3-Chloro-4-hydroxy-phenyl)-carbamic acid phenyl ester

The compound was obtained in 46% yield (32.1 mg) using the protocol described in method F.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  = 2.38 (s, 3 H), 6.76 (s, 1H), 7.15 (m, 5H), 7.32 (m, 2 H). NMR-<sup>13</sup>C (DMSO-d<sub>6</sub>)  $\delta$  = 16.5, 109.1, 115.2, 118.8, 126.7, 128.5, 129.5, 129.7, 139.4, 153.4, 157.4

Example 31: (3,5-Dibromo-4-hydroxy-phenyl)-carbamic acid phenyl ester

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The compound was obtained in 25 % yield (10.2 mg) using the protocol described in method F.

NMR- $^{1}$ H (DMSO- $^{1}$ d<sub>6</sub>)  $\delta$  = 7.33 (m, 2 H), 7.45 (m, 2H), 7.50 (s, 2H)

Example 32: (3,5-Dichloro-4-hydroxy-phenyl)-carbamic acid 2-isopropyl-5-methyl-cyclohexyl ester

According to method G 4-amino-2,6-dichloro-phenol (40 mg, 1 eq) and (-)-menthylchloroformate (54  $\mu$ l, 1.1 eq) in DCM gave 44.1 mg (54 %) of the title compound as a white solid.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  = 0.71 (d, 3H), 0.78-0.96 (m, 7H), 0.99-1.16 (m, 2H), 1.29-1.58(m, 2H), 1.59-1.71 (m, 2H), 2.0-2.15 (m, 2H), 4.58 (m, 1H), 7.49 (s, 2H), 9.68 (s, 1H), 9.73 (s, 1H)

Example 33: (3,5-Dichloro-4-hydroxy-phenyl)-carbamic acid hexyl ester

According to method G 4-amino-2,6-dichloro-phenol (40 mg, 1 eq) and hexylchloroformate (41  $\mu$ L, 1.1 eq) gave 30 mg (43 %) of the title compound as a white solid.

NMR-<sup>1</sup>H (DMSO-d<sub>6</sub>)  $\delta$  = 0.75 (m, 3H), 1.21-1.40 (m, 6H), 1.48-1.62 (m, 2H), 4.22 (m, 2H), 7.32 (s, 2H), 9.69 (s, 1H), 9.75 (s, 1H).

Example 34: 1-[3-Chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-3-(2-trifluoromethyl-phenyl)-urea

According to method J 1-(3-amino-5-chloro-4-hydroxy-phenyl)-3-cyclohexyl-urea (30 mg, 0.11 mmol) and 1-isocyanato-2-trifluoromethyl-benzene (21 mg, 0.11 mmol) gave 1-[3-chloro-5-(3-cyclohexyl-ureido)-2-hydroxy-phenyl]-3-(2-trifluoromethyl-phenyl)-urea (16 mg, 31%).

NMR- $^{1}$ H (DMSO- $^{1}$ d<sub>6</sub>)  $\delta$  0.98-1.28 (m, 5 H), 1.39-1.76 (m, 5 H), 3.30-3.42 (m, 1 H), 5.84 (d, J = 7.8 Hz, 1 H), 7.24 (d, J = 7.8 Hz, 1 H), 7.31 (d, J = 2.4 Hz, 1 H), 7.52-7.67 (m, 2 H), 7.71-7.75 (m, 2 H), 8.20 (br. s, 1 H), 8.80-8.82 (m, 1 H), 8.97-9.04 (m, 1 H), 9.11 (s, 1 H); MS: m/z: 471.1 [M+H $^{+}$ ].

# Example 35: Specificity of inhibition of certain enzymes by compounds according to the present invention

In order to characterize the specificity of various compounds the following assays were performed. PPIase activity of hPin1, hCyp18, LpCyp18, hFKBP12 and EcParvulin was measured using the protease-coupled PPIase assay according to Fischer et al. (Fischer, G.; Bang, H.; Mech, C. Determination of enzymatic catalysis fort he cis-trans-isomerization of peptide binding in proline-containing peptides. [German] Biomed. Biochem. Acta 1984, 43, 1101-1111; Hennig et al., Selective Inactivation of Parvulin-like peptidyl-prolyl cis/trans isomerases by Juglon, Biochemistry. 1998, 37(17):5953-5960). For hPin1 measurements Ac-Ala-Ala-Ser(PO<sub>3</sub>H<sub>2</sub>) -Pro-Arg-pNA was used as a substrate and trypsin (final concentration

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190 μg/ml) as an isomer-specific protease. Activity measurements of other PPIases were made with the substrate peptide Suc-Ala-Phe-Pro-Phe-pNA and the protease -chymotrypsin (final concentration 470 μg/ml). The assays were performed in a final reaction volume of 150 μl at final concentrations of 6 nM hPin1, 10 nM hCyp18, 5 nM LpCyp18, 20 nM EcParvulin and 20 nM hFKBP12, respectively, and 120 μM substrate peptide in 35 mM HEPES (pH 7.8). For inhibition experiments 100-0.01 μM of effector freshly diluted from a DMSO stock solution were added. The amount of solvent was kept constant within each experiment, usually below 0.3% (v/v). All reactions were started by addition of protease. The test was performed by observing the released 4-nitroaniline at 390 nm with a MR5000 UV/Vis spectrophotometer (Dynex) at 6°C. Data were evaluated by calculation of pseudo-first-order rate constants k<sub>obs</sub> in presence of PPIase and PPIase/effector, respectively, and corrected for the contribution of the non-catalyzed reaction (k<sub>0</sub>). Inhibition constants IC<sub>50</sub> were calculated using SigmaPlot 8.0 (SPSS).

The following target enzymes which are all rotamases belonging to different classes of rotamases were used:

- T-1: Protein interacting with NIMA (-kinase), hPin1
- T-2: First described human Rapamycin receptor, hFKBP12
- T-3: Human Cyclosporin A receptor with 18 kDa molecular weight, hCyp18
- T-4: Leishmonia pneumophila virulence Cyclosporin A receptor with 18 kDa molecular weight, LpCyp18
- T-5: Bacterial Juglon sensitive non proteolytic enzyme, EcParv

These rotamases are known in the art. Their production and characteristics may be taken from the following references.

# Review about all PPIase families

Gothel, S. F.; Marahiel, M. A. TI Peptidyl-prolyl cis-trans isomerases, a superfamily of ubiquitous folding catalysts [Review]. Cell. Molec. Life Sci. 1999, 55, 423-436

#### Pin1

Lu, K. P.; Hanes, S. D.; Hunter, T. (1996) A human peptidyl-prolyl isomerase essential for regulation of mitosis. *Nature* 1996, 380, 544-547

Yaffe, M. B.; Schutkowski, M.; Shen, M. H.; Zhou, X. Z.; Stukenberg, P. T.; Rahfeld, J. U.; Xu, J.; Kuang, J.; Kirschner, M. W.; Fischer, G.; Cantley, L. C.; Lu K. P. SEQUENCE-SPECIFIC AND PHOSPHORYLATION-DEPENDENT PROLINE ISOMERIZATION - A POTENTIAL MITOTIC REGULATORY MECHANISM. Science 1997, 278, 1957-1960

Shen, M.; Stukenberg, P. T.; Kirschner, M. W.; Lu, K. P. The essential mitotic peptidyl-prolyl isomerase Pin1 binds and regulates mitosis-specific phosphoproteins. *Genes Developm.* 1998, 12, 706-720.

#### **EcParvulin**

Rahfeld JU. Schierhorn A. Mann K. Fischer G. A novel peptidyl-prolyl cis/trans isomerase from Escherichia coli. FEBS Letters. 1994, 343, 65-69

Rahfeld JU. Rucknagel KP. Schelbert B. Ludwig B. Hacker J. Mann K. Fischer G. Confirmation of the existence of a third family among peptidyl-prolyl cis/trans isomerases. Amino acid sequence and recombinant production of parvulin. *FEBS Letters.* 1994, 352, 180-184

#### FKBPs (including FKBP12) and Cyclophilins (including Cyp18)

For recent reviews on cyclophilins and FKBPs and their effectors, see: (a) Fischer, G. Peptidyl-prolyl cis/trans isomerases and their effectors. Angew. Chem., Int. Ed. Engl. 1994, 33, 1415-1436. (b) Galat, A.; Metcalfe, S. M. Peptidylproline cis/trans isomerases. Prog. Biophys. Molec. Biol. 1995, 63, 67-118.

#### LpCyp18

Schmidt B. Tradler T. Rahfeld JU. Ludwig B. Jain B. Mann K. Rucknagel KP. Janowski B. Schierhorn A. Kullertz G. Hacker J. Fischer G. A cyclophilin-like peptidyl-prolyl cis/trans

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isomerase from Legionella pneumophila--characterization, molecular cloning and overexpression. *Mol. Microbiol.* 1996, 21,1147-1160

In order to cluster the various rotamase inhibitors the following classes were defined with "A" indicating the most potent rotamase inhibitor.

A: IC50 < 1  $\mu$ M

B:  $1 \mu M < IC50 < 10 \mu M$ 

C:  $10 \,\mu\text{M} < \text{IC}50 < 50 \,\mu\text{M}$ 

D:  $50 \mu M < IC50 < 100 \mu M$ 

E:  $IC50 > 100 \mu M$ 

Table 2

Specificity of the inhibition with rotamases

A: IC50 < 1  $\mu$ M

B:  $1 \mu M < IC50 < 10 \mu M$ 

C:  $10 \mu M < IC50 < 50 \mu M$ 

D:  $50 \mu M < IC50 < 100 \mu M$ 

E: IC50 > 100  $\mu$ M

Table 2
Specificity of the inhibition with rotamases

	N°			Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI OH N	120	С	D	С	Е	-

	N°			Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI CI	.655	. C	E	Е	E	С
CI CI CI	512	С	E	D	E	С
CI SO2	563	В	В	E ·	Е	E
CI CI	109	A	E	С	E	С
C C C C C C C C C C C C C C C C C C C	599	В	Е	E	D	С
CI CI	118	В	D	C	С	В
	643	С	Е	E	Е	E
HO CI	605	A	Е	С	E	В

	N <sub>o</sub>			Target		
Compound		T-1	T-2	T-3	T-4	T-5
OH HN S	<u>.</u> 266	<b>A</b>	E	E	E	В
CI CI	629	A	E	С	E	В
CI CI	102	В	E	C .	С	В
CI CI CI	30	В	E	E	Е	E
CI S CF3	264	A	-	-	-	<u>-</u>
OH H H	254	A	-	· <b>-</b>	-	-
CI N S	639	A	<b>-</b>	-	-	-

	No			Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI S N	640	В	-	-	-	-
CI SI	257	<b>A</b>	-	-	-	
F H H H	126	A	-	-	-	-
F N N N	127	В	-	-	-	-
F OH I I I	142	A	-	• ·	•	-
CI CI	31	A	-	-	-	-
CI CI	593	В	-	-	-	-

_	No			Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI N IN	637	В	-	-	-	<del>-</del>
CI S N	638	В	-	_ :	-	-
CI N N	636	A	-	-	-	-
CI NH HN NH	622	A	-	· -	-	-
CI HN N	656	Α.	•	-	-	-

Commenced	N°			Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI CI CI	.371	A	E	С	E	C
HO CI	672	A	С	В	. <b>C</b>	С
CI OH II	647	В	Е	E	E	E
ĕ T C C C C C C C C C C C C C C C C C C	483	В	Е	С	E	D
OH TO	482	В	Е	C	E	E
OH H S	343	В	E	С	E	Е

Commi	N°			Target		
Compound		T-1	T-2	Т-3	T-4	T-5
CI S CI	441	В	E	С	В	E
F OH IN S	399	A	E	D	D	C
OH HN S	610	A	-	-	-	-
CI OH I OH CI	673	A	-	-	-	-
F NO <sub>2</sub>	400	A	-		-	
CI HO CI	719	A	E	D	С	-
CI HO CI	703	A	Е	Е	E	В

	N°			Target		
Compound		T-1	T-2	T-3	T-4	T-5
CI HO CI	.700	A	E	E	Е	С
CI HO CI	710	A	E	В	E	E
CI HO CI	716	В	<b>E</b> .	E	E	С
CI HO CI	1273	A	E	E	Е	В
CI HO CI	1293	В	E	E	E	С
CI NO2	1294	A	Е	E	E	В
CI HO CI	894	A	E	E	E	В
HO CI	1295	В	Е	E	E	В

	N°			Target		
Compound		T-1	T-2	T-3	T-4	T-5
HO CI	1296	В	E	C	E	C
CI HO CI	1297	A	E	E	E	C
CI CI	1298	A	Е	E	E	С
CI HO CI	1299	A	Е	A	E	С
HO CI	1044	<b>A</b>	С	C	В	С

As may be taken from the above table 2 the following compounds 24, 88, 89, 110, 169, 170, 298, 342, 344, 377, 378, 700, 703, 710, 894, 1273, 1294, 1297 are of class A and are thus extremely specific for hPin1.

# Example 36: Specificity of inhibition of proteases

In order to investigate the impact of some of the inventive compounds on the activity of key proteases the following assay was performed: Protease activities were measured

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spectrophotometrically at 30°C according to Schomburg and Salzmann (Schomburg, B.; Salzmann M. GBF: Enzyme Handbook. Springer Verlag, Berlin Heidelberg, 1991) and Bergmeyer et al. (Bergmeyer, H. U.; Bergmeyer, J.; Graßl, M. Methods of Enzymatic Analysis, Vol. V Enzymes 3: Peptides, Proteinases and Their Inhibitors. pp 55 – 371, VCH, Weinheim, 1988). The release of 4-nitroaniline was determined at 390 nm with a Spectramax Plus UV/Vis spectrophotometer (Molecular Devices). The cathepsin B assay was performed in a reaction mixture containing 0.2 μg/ml cathepsin B, 2 mM Z-Arg-Arg-pNA in 88 mM KH<sub>2</sub>PO<sub>4</sub>, 12 mM Na<sub>2</sub>HPO<sub>4</sub>, 1.33 mM EDTA, 0.03% Brij 35 (pH 5.8). The trypsin assay was carried out in a reaction mixture containing 0.1 μg/ml trypsin and 120 μM Ac-Ala-Ala-Ser(PO<sub>3</sub>H<sub>2</sub>) -Pro-Arg-pNA in 35 mM HEPES (pH 7.8) and the papain assay in a mixture consisting of 16 μg/ml papain and 2 mM Bz-DL-Arg-pNA in 10 mM Na<sub>2</sub>HPO<sub>4</sub>, 2 mM L-Cys, 5 mM EDTA (pH 6.5). In general, reactions were started by addition of peptide substrate after a 30 min incubation of 1-100 μM effector with given concentrations of enzyme.

The key proteases used were the following:

T-6: Papain

T-7: Trypsin

T-8: Cathepsin

In order to cluster the various compounds the following classes of activity were defined.

A:  $IC50 < 1 \mu M$ 

B:  $1 \mu M < IC50 < 10 \mu M$ 

C:  $10 \mu M < IC50 < 50 \mu M$ 

D:  $50 \mu M < IC50 < 100 \mu M$ 

E:  $IC50 > 100 \mu M$ 

Table 3
Specificity of the inhibition of some proteases

	N°		Target	
Compound		T-6	T-7	T-8

	N°		Target	
Compound	_	T-6	T-7	T-8
CI NOT	102	D ·	С	D
CI THE THE	109	E	-	-
CI OH I	118	E	-	-
OH H H	643	E	-	-
CI CI CF3	264	E	E	E
CI SO2	563	E	-	<u>.</u>
CI CI CI	371	E	-	-
CI CI CI	599	E	-	D

	N°		Target	
Compound		T-6	T-7	T-8
CI OH II	645	E	-	-
CI OH	497	E	<b>.</b>	C
CI CI	644	E	-	-
OH OH	646	E	-	Е
CI CF3	649	В	-	D <sub>.</sub>
OH TO CO	498	E	-	-

	N°		Target	<del></del> ge <b>t</b>		
Compound		T-6	T-7	T-8		
CI H	499	E	-	_		
CI OH II S	343	E	<b>-</b>	-		
CI SCI	441	Е	-	-		
P N S	385	E	-	-		
OH S S CI	399	E	-	C.		
HO CI	1296	E	Е	E		
CI HO CI	1273	E	E	Е		

	N°		•	
Compound		T-6	T-7	T-8
CI NO TO THE PART OF THE PART	703	E	D	E
CI HO CI .	710	E	-	-
HO CI	716	E	-	· <b>-</b>

As may be taken from table 3 none of the tested compound is a strong inhibitor of any of the key proteases tested.

## Example 37: Cytotoxic effects on tumor cell lines

In order to show that the compounds according to the present invention are actually useful in the treatment of tumors, the cytotoxic effects of some of said compounds on tumor cell lines were determined.

For this cytotoxic evaluation of the compounds the commercial available WST-1 assay (Roche) was used according to the manufacturer's instructions. The assay is based on the cleavage of the tetrazolium salt WST-1 by mitochondrial dehydrogenases found in viable cells. In general compounds were added to cells cultured in 96-well plates at 37°C. After 48 h of incubation 10  $\mu$ l of WST-1 solution was added. The formazan dye was analyzed with an ELISA plate reader at (450 vs. 620) nm.

The following tumor cell lines were used in this assay:

CL-1: human acute myeloid leukemia, HL-60

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CL-2: human cervix carcinoma, HeLa

CL-3: human prostate carcinoma, PC-3

CL-4: human colon adenocarcinoma, Caco-2

CL-5: human breast adenocarcinoma, MCF-7

In order to cluster the efficacy of the various compounds the following classes in terms of EC50 were defined.

A: EC50 < 10  $\mu$ M

B:  $10 \mu M < EC50 < 50 \mu M$ 

 $C:.50 \mu M < EC50 < 100 \mu M$ 

D:  $100 \mu M < EC50 < 200 \mu M$ 

E: EC50 > 200  $\mu$ M

Table 4 Cytotoxic effects on tumor cell lines

	N°	Target					
Compound		CL-1	CL-2	CL-3	CL-4	CL-5	
CI NOH NO	102	A	A	<b>A</b>	A	, <b>A</b>	
OH S S CF₃	261	A	В	В	В	В	
CI S CF3	264	A	A	A	A	A	

	N°	Target						
Compound		CL-1	CL-2	CL-3	CL-4	CL-5		
CI SI	109	В	A	В	-	A		
CI S S	254	В	В	В	-	В		
CI OH N	30	A		-	A	-		
CI H H CF3	221	В	-	-	-	В		
	6	В	-	-	-	A		
CI N N N	54	В	-	<del>-</del> .	-	A		
F OH	150	В	-	-	-	A		

	N° Target					
Compound		CL-1	CL-2	CL-3	CL-4	CL-5
OH HZ S	639	A	-	-	-	<b>B</b>
OH H H	640	В	· -	-	-	В
CI N	653	A	-	<b>-</b>	-	В
CI S S	629	A	A	Α.	-	A
CI OH II	645	A	<b>A</b> .	A	-	A

_	N°			Target		
Compound		CL-1	CL-2	CL-3	CL-4	CL-5
OH H S	329 .	В	В	В	-	В
CI CI OMe	493	В	<b>A</b>	<b>A</b>	-	-
CI OH II	484	В	A	A	-	-
CI CI	483	-	В	В	-	-
F OH S S CI	399	<b>A</b>	A	A.	-	A
OH HZ S	654	-	В	-	-	A

	N°		Target						
Compound		CL-1	CL-2	CL-3	CL-4	CL-5			
F OH II S	357 .	<b>A</b>	A	A	-	-			
OH OH S	413	В	A	В	-	-			
P H S CI	402	В	В	В	-	-			
CI CI CI	332	B <sub>.</sub>	В	В	-	-			
OH H S	630	В	A	<b>A</b>	-	-			
P N S CI	403	В	A	A	-	-			

	N°	Target				
Compound		CL-1	CL-2	CL-3	CL-4	CL-5
DH ZZ O H	631	A	-	В	-	
OH CI S CI	632	A	- -	В	- -	-
CI HN CI	633	A	-	A	-	-
	673	-	-	-	-	A

	N°		Target					
Compound		CL-1	CL-2	CL-3	CL-4	CL-5		
CI HN S CI	652	<b>A</b>	ı	<b>A</b>	-	<del>-</del> -		
HO CI	1273	В	· C	В	В	-		
сі Но	703	В	В	В	В	-		
HO CI	1296	С	<del>.</del>	-	-	-		
CI HO CI	1297	С	-		-	-		
HO S CI	1044	В	В	В	-	-		

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As may be taken from table 4 all of the tested compounds are highly efficient in exhibiting a cytotoxic effect on at least one of the various tumor cell lines tested. Of particular relevance are compounds 102, 264, 357, 399, 629, 633, 645, 652, 673, 703, 1044, 1273.

# Example 38: FACS measurements and TUNEL assay

In order to show that the compounds according to the present invention are actually useful for inducing apoptosis in tumor cells, FACS measurements and TUNEL assay were performed. Enari M. Sakahira H. Yokoyama H. Okawa K. Iwamatsu A. Nagata S. A caspase-activated DNase that degrades DNA during apoptosis, and its inhibitor ICAD [erratum appears in Nature 1998 May 28;393(6683):396.]. Nature. 391:43-50, 1998

Darzynkiewicz Z. Juan G. Li X. Gorczyca W. Murakami T. Traganos F. Cytometry in cell necrobiology: analysis of apoptosis and accidental cell death (necrosis). Cytometry. 27:1-20, 1997

Apoptotic HL-60 cells were detected by FACS analysis of FITC-dUTP-labelled DNA breaks using the Apo-Direct kit (BD-Pharmingen) according to the manufacturer's protocol.

As may be taken from Fig. 2 compounds 102 and 264 induce apoptosis in tumor cells.

## Example 39: Cyclin D1 down regulation

In order to show that the compounds according to the present invention are actually acting the expected way and induces cyclin D1 down regulation, cyclin D1 marker analysis were performed

MCF-7 (5×10<sup>5</sup> cells/well) and HeLa cells (1.5×10<sup>5</sup> cells/well) were seeded in 6-well plates and incubated at 37°C over night. Compounds or DMSO (final solvent concentration 0.1%) were added to the cells and incubated for different times as indicated. Subsequently, cells were lysed in RIPA buffer for 30 min on ice and centrifuged for 20 min at 4°C. After addition of electrophoresis sample buffer (4×) and 50 mM DTT to the supernatant, samples were

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boiled for 4 min at 95°C. Samples (equivalent to 2×10<sup>5</sup> cells/well) were run on a 15% SDS gel followed by blotting onto PVDF membrane.

The membrane was blocked for 1 h in 10 mM Tris (pH 7.5), 100 mM NaCl, 0.1% Tween-20 and 5% non-fat dry milk (blocking buffer) and incubated for 1 h with mouse anti-hCyclin D1 monoclonal antibody (clone DCS-6, BD Biosciences) diluted to 1  $\mu$ g/ml in blocking buffer. Blots were washed 3 × 10 min with 10 mM Tris (pH 7.5), 100 mM NaCl, 0.1% Tween-20 (washing buffer) and incubated with 0.7  $\mu$ g/ml peroxidase-conjugated sheep anti-mouse IgG (Sigma) in blocking buffer for 1 h. After washing 3 × 10 min with washing buffer, the plot was developed with the ECL+ detection kit (Amersham Biosciences).

Of particular relevance are compounds 30, 102, 264, 399, 629, 639, 657, 673.

Example 40: DAPI staining

In order to show that the compounds according to the present invention are actually useful for inducing apoptosis in tumor cells, DAPI staining was performed.

Hela cells grown on poly-L-Lys-coated coverslips were fixed with 2% paraformaldehyde/MeOH.

Cellular DNA was stained with DAPI staining buffer (100 mM Tris (pH 7.4), 150 mM NaCl, 1 mM CaCl2, 0.5 mM MgCl2, 0.1% nonidet P-40, 1 µg/ml DAPI (Molecular Probes)). All the steps were performed at room temperature, and cells were washed two times with PBS after each step. Finally, cells were mounted in 80% glycerol/PBS.

As may be taken from Fig. 3 compounds 30, 102, 264 and 399 induce apoptosis in tumor cells.

The features of the present invention disclosed in the specification, the claims and/or the drawing may both separately and in any combination thereof be material for realizing the invention in various forms thereof.